Task 2 Report

SENSITIVITY ANALYSES OF THE SEPTEMBER 8-11, 1993 OZONE EPISODE

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1. INTRODUCTION

The TNRCC is responsible for developing a State Implementation Plan (SIP) for ozone in Houston/Galveston and Beaumont/Port-Arthur (HGBPA) ozone nonattainment areas (the Houston area). The TNRCC's SIP relies upon photochemical modeling to relate atmospheric ozone concentrations to emission levels for ozone precursors. The most recent modeling was performed using the Comprehensive Air Quality Model with extensions (CAMx) version 2.03 for the December, 2000 SIP revision and considered emissions of volatile organic compounds (VOCs), nitrogen oxides (NOx) and carbon monoxide. Since then a number of new features have been implemented in the CAMx modeling system, in particular, flexi-nesting and chlorine chemistry. Recent studies (ENVIRON, 2001; Tanaka, 2000) have suggested that reactive chlorine compounds may play a significant role in ozone formation in the Houston atmosphere, while the implementation of the flexi-nesting features of the CAMx model may result in significant impacts for the Houston area with respect to model performance. In addition, during the summer of 2000 the Texas Air Quality Study (TexAQS) was conducted to collect atmospheric measurements of ozone and ozone precursors in order to further support atmospheric computer modeling of the Houston area as well as to better characterize industrial precursor emissions within the area. The purpose of this study is to apply new features of the CAMx model to the 8-11 September, 1993 ozone episode and to evaluate model performance under alternative emission scenarios. In addition, the modeling effort will focus on the determination of alternative VOC emission reduction scenarios which would be required to compensate for the NOx reductions currently implemented in the future year Strategy I8a. Although the final SIP was based on the Strategy I8 emission inventory, Strategy I8a is used here as it includes a minor correction to the Strategy I8 inventory.

Objectives

The overall objectives of this study are as follows:

1. Apply new features of the CAMx model to the 8-11 September, 1993 ozone episode and ~~to~~ evaluate model performance. The latest version of CAMx, version 3.01, is applied and compared with the modeling results using CAMx version 2.03, which was used in the 2000 SIP revision. Both the flexi-nesting and chlorine chemistry features of CAMx version 3.01 are then applied and model performance evaluated using the statistical and graphical analyses recommended by EPA Guidance.

2. Perform sensitivity analyses in order to assess model performance under alternative emissions scenarios. The various alternative emission scenarios are developed to reflect a realistic estimate of VOC emission levels consistent with the TexAQS analysis. Adjustments to the VOC emission inventory are made based on the TexAQS Special Inventory and upset/maintenance reports compiled from EPA Region 12 databases in order to characterize the types of non-routine emissions which are known to occur in the industrial areas.

3. Determine the level of VOC emission reductions necessary to achieve the same peak ozone levels as Strategy I8a and the necessary VOC emission reductions required to compensate for the remaining NOx emission reductions.

This report documents and discusses the CAMx modeling performed to achieve the first objective listed.

2. TECHNICAL APPROACH

This section of the report documents the Houston ozone modeling databases that were utilized, the various versions and new features of the CAMx model used to perform the sensitivity simulations, and the implementation of the CAMx model.

CAMx MODELING DATABASES

The TNRCC has developed CAMx modeling databases for ozone episodes that occurred in 1993 during the COAST field study. The episode periods are September 6-11 and August 16-20, 1993. Several concerns have been raised about the performance of modeling using these databases, and the TNRCC did not use the August episode in the HGBPA SIPs (the TNRCC is currently developing new modeling episodes). The TNRCC has also performed Houston modeling over a much larger area referred to as the SuperCOAST domain. The modeling performed for the current study utilizes the SuperCOAST domain with an inner 2-way nested 4-km grid which is the same as the 4-km grid used in the original COAST domain. The impacts due to a high-resolution 1.33-km flexi-nested grid are investigated within a sub-region encompassing the industrial areas along the Houston Ship Channel and Galveston Bay. The area covered by the CAMx model for the SuperCOAST domain is shown in Figure 2-1. The domain has an outer 16-km grid with an inner 2-way nested 4-km grid. The grid is defined in UTM zone 15 coordinates and has 8 vertical layers between the surface and 3.03 km. with a surface layer 20 meters deep. Figure 2-2 displays the location of the 1.33-km grid within the 4-km HGBPA grid.

The COAST domain meteorological fields for both the August and September 1993 episodes were developed using the SAIMM hydrostatic meteorological model with data assimilation (Kessler and Douglas, 1992). SAIMM was applied with relatively strong assimilation of wind data in an attempt "nudge" the model into reproducing the timing and magnitude of the land/sea breezes (Lolk et al., 1995). This has raised some concerns that the strength of the nudging may have compromised the consistency of the meteorological fields (Yocke et al., 1996). Recent studies have developed alternate meteorological fields for the September Episode using the Regional Atmospheric Modeling System (RAMS) at 4 km resolution (Emery et al., 2001), and alternate meteorological fields using the PSU/NCAR Mesoscale Model version 5 (MM5) at 4 km resolution (ENVIRON and MRC, 2001), including an investigation of meteorological modeling at very fine resolution (1.33 km) using RAMS and MM5. CAMx modeling and performance evaluations utilizing these meteorological databases have been performed and documented for the September 1993 ozone episode in Tesche and McNally, 2001.

The emission inventories were developed by the TNRCC and have undergone continual upgrades to include the latest information. The inventories for the September episode are more updated than for the August episode because the September episode continues to be used for SIP modeling. For example, the biogenic emissions were updated based on new local surveys and the latest emission factors as described in Yarwood et al., (1999). The biogenic emission inventories were prepared using the GLOBEIS model (http://www.globeis.com).

The anthropogenic point, area, and nonroad mobile emission inventories were prepared using SMOKE (http://envpro.ncsc.org/products/smoke/), while the on-road mobile source emissions were processed using Fast-EPS. Boundary and initial conditions were developed by the TNRCC using a regional scale model (Yocke et al., 1996).

The chlorine emission inventory used for this study was prepared by UT and is described in detail elsewhere (Tanaka and Allen, 2001). Briefly, the inventory included the following source types:

- Point sources included in the TNRCC's point source database (PSDB) and the Toxic Release Inventory (TRI).
- Emissions from chlorinating swimming pools.
- Emissions from chlorinating large cooling towers.
- Formation of chlorine from sea salt reactions in the atmosphere.

The chlorine emission estimates provided by UT were processed using the emissions preprocessor system version 2 (EPS2) and formatted for CAMx. For simplicity, UT represented all emissions as point sources (e.g., area source emissions such as swimming pools were broken out by grid cell and represented as a single point source released at the surface in the center of the appropriate grid cell). Thus, only the point source emission file for CAMx was modified by the inclusion of chlorine sources - the area source emission files did not change from the base case. The chlorine point sources were merged with the VOC, NOx and CO point sources for the SuperCOAST domain. The chlorine emission inventory used for the resent modeling effort is documented and discussed in more detail (including limitations) elsewhere (ENVIRON, 2001).

The TNRCC provided the CAMx input files for the September 1993 episodes while the simulation control files were provided by MCNC. To document the input data that were used, the CAMx control files for the first day of the September 1993 episode for CAMx version 2.03 and version 3.01 are shown in Figures 2-3 and 2-4, respectively.

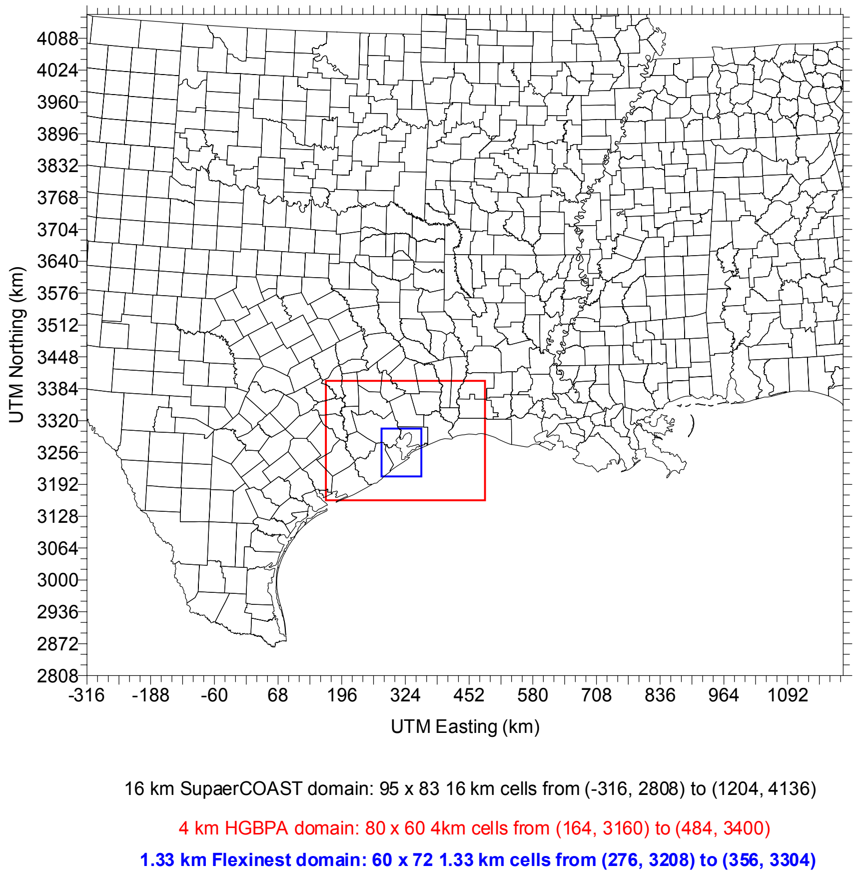

Figure 2-1. Map of the SuperCOAST domain showing the location of the 4-km HGBPA and 1.33 km Flexi-nest domains.

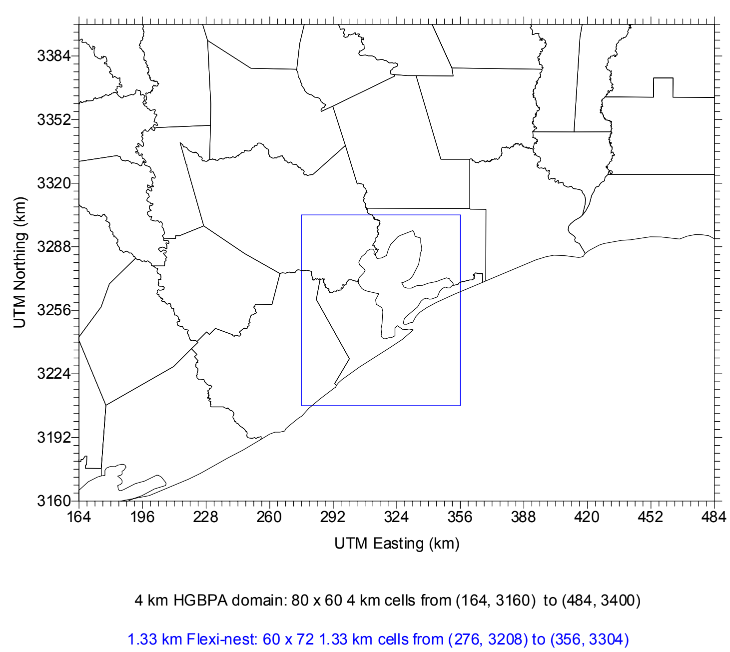

Figure 2-2. Map of the 4-km HGBPA domain showing the location of the 1.33-km Flexi-nest grid.

```
CAMx SuperCOAST aak93 : one HG/BPA 4x4km subgrid, 930906 V2.03 (ENVIRON 12/27/01)
Root output name    |../../output/aak93/camx2/camx2.930906.aak93
Start time/date     |1993 09 06    0.
End time/date       |1993 09 06 2400.
DT:max,in,emis,out  |0.5 1. 1. 1.
nx,ny,nz            |95  83  8
Coordinate ID       |UTM
xorg,yorg,dx,dy,uzn|-316. 2808.  16.  16.  15
time zone           |6
PiG parameters      |2000. 12.
Avg output species  |23
                    |NO        NO2       O3        OLE       PAN       NXOY
                    |PAR       TOL       XYL       FORM      ALD2      ETH
                    |CRES      MGLY      OPEN      PNA       CO        HONO
                    |H2O2      HNO3      ISOP      MEOH      ETOH
Num fine nest       |1
net grid params     |31 50 23 37  8  4
SMOLAR or BOTT?     |SMOLAR
Restart             |false
Chemistry           |true
Dry dep             |true
Wet dep             |false
PiG submodel        |true
Staggered winds     |false
Treat area emiss    |true
Treat point emiss   |true
1-day emiss inputs  |true
3-D average file    |true
Source Apportion    |false
Chemparam           |../../input/common/CAMx2.chemparm.3
Photolysis rates    |../../input/common/camx_photorate.930906-
930911.isop.tcas_16km+hgbpa_04km.better
Landuse             |../../input/common/uamv_landuse.super_16km
Height/pressure     |../../input/met/uamv_zp.930906.tcas_16km
Wind                |../../input/met/uamv_wind.930906.super_16km.CAMx2
Temperature         |../../input/met/uamv_temp.930906.super_16km.CAMx2
Water vapor         |../../input/met/uamv_h2o.930906.super_16km
Cloud cover         |
Rainfall            |
Vertical diffsvty   |../../input/met/uamv_kv.930906.super_16km
Initial conditions  |../../input/common/camx2.930905.93basAj.ic.bin
Boundary conditions|../../input/bc-ic-tc/93basAj/uamv_bc.930906
Top concentration   |../../input/bc-ic-tc/93basAj/uamv_tc.clean
Albedo/haze/ozone   |../../input/common/uamv_aho.930906-930911.tcas_16km+hgbpa_04km
Point emiss         |../../input/emiss/aak93/egts.allpts.19930906.93b.super.bin
Area emiss          |../../input/emiss/aak93/low_ei.super16km.19930906.93babb.bin
Landuse          #1 |../../input/common/uamv_landuse.hgbpa_04km
Height/pressure  #1 |../../input/met/uamv_zp.930906.hgbpa_04km
Wind             #1 |../../input/met/uamv_wind.930906.hgbpa_04km.CAMx2
Temperature      #1 |../../input/met/uamv_temp.930906.hgbpa_04km.CAMx2
Vertical diff    #1 |../../input/met/uamv_kv.930906.hgbpa_04km
Area emiss       #1 |../../input/emiss/aak93/low_ei.4km.19930906.93babb.bin
Coarse grid restart|
Fine grid restart   |
PiG restart         |
```

Figure 2-3. CAMx (Version 2.03) control file (CAMx.in) for the first day of the September 1993 episode.

```
Version              |VERSION3
Message string       |CAMx SuperCOAST aak93 : one HG/BPA 4x4km subgrid, 930906 V3.01
(ENVIRON 12/27/01)
Root output name     |../../output/aak93/camx3/camx3.930906.aak93
Start time/date      |1993 09 06    0.
End time/date        |1993 09 06 2400.
DT:max,in,emis,out   |0.5 1. 1. 1.
nx,ny,nz             |95  83  8
Coordinate ID        |UTM
xorg,yorg,dx,dy,uzn|-316. 2808.  16.  16.  15
time zone            |6
PiG parameters       |2000. 12.
Avg output species   |1
                     |O3
Num fine nest        |1
net grid params      |31 50 23 37  8  4
SMOLAR or BOTT?      |SMOLAR
Solver               |CMC
Restart              |false
Chemistry            |true
Dry dep              |true
Wet dep              |false
PiG submodel         |true
Staggered winds      |false
Treat area emiss     |true
Treat point emiss    |true
1-day emiss inputs   |true
3-D average file     |false
Source Apportion     |false
Chemparam            |../../input/common/CAMx3.chemparm.3
Photolysis rates     |../../input/common/camx_photorate.930906-
930911.isop.tcas_16km+hgbpa_04km.better
Landuse              |../../input/common/uamv_landuse.super_16km
Height/pressure      |../../input/met/uamv_zp.930906.tcas_16km
Wind                 |../../input/met/uamv_wind.930906.super_16km.CAMx2
Temperature          |../../input/met/uamv_temp.930906.super_16km.CAMx2
Water vapor          |../../input/met/uamv_h2o.930906.super_16km
Cloud cover          |
Rainfall             |
Vertical diffsvty    |../../input/met/uamv_kv.930906.super_16km
Initial conditions   |../../input/common/camx2.930905.93basAj.ic.bin
Boundary conditions|../../input/bc-ic-tc/93basAj/uamv_bc.930906
Top concentration    |../../input/bc-ic-tc/93basAj/uamv_tc.clean
Albedo/haze/ozone    |../../input/common/uamv_aho.930906-930911.tcas_16km+hgbpa_04km
Point emiss          |../../input/emiss/aak93/egts.allpts.19930906.93b.super.bin
Area emiss           |../../input/emiss/aak93/low_ei.super16km.19930906.93babb.bin
Landuse           #1 |../../input/common/uamv_landuse.hgbpa_04km
Height/pressure #1   |../../input/met/uamv_zp.930906.hgbpa_04km
Wind              #1 |../../input/met/uamv_wind.930906.hgbpa_04km.CAMx2
Temperature       #1 |../../input/met/uamv_temp.930906.hgbpa_04km.CAMx2
Vertical diff     #1 |../../input/met/uamv_kv.930906.hgbpa_04km
Area emiss        #1 |../../input/emiss/aak93/low_ei.4km.19930906.93babb.bin
Coarse grid restart|
Fine grid restart    |
PiG restart          |
```

Figure 2-4. CAMx (version 3.01) control file (CAMx.in) for the first day of the August 1993 episode.

CAMx MODEL VERSIONS

The TNRCC SIP modeling simulations for the 1993 ozone episodes were performed using the Comprehensive Air Quality Model with extensions (CAMx) version 1.13. ENVIRON subsequently performed a comparison of the 2007 future year scenario using CAMx versions 1.13 and 2.03 (ENVIRON, 2000). The comparison study resulting in small differences in the modeled ozone between CAMx v1.13 and v2.03 with differences in the daily maximum ozone on the order of 1 ppb. Subsequently, the TNRCC revised the SIP modeling demonstrations using CAMx version 2.03 and developed the December 2000 SIP revision. The starting point of the model sensitivity simulations documented herein is the CAMx version 2.03 as implemented by the TNRCC for the December 2000 SIP revision. The version of the code used in this study was obtained from the CAMx web site http://www.camx.com.

Since the development of the TNRCC SIP scenarios, several updates and enhancements have been made to the CAMx model. Most notably, in January 2001, ENVIRON released version 3 of the CAMx model. The primary differences in model versions affecting the simulations performed include an improved vertical transport scheme and the inclusion of the flexi-nesting capabilities. With the implementation of flexi-nesting, high resolution nested grids may be introduced into the model simulation at any time during the episode, allowing for more computational efficient model applications for nested grids. Other minor coding modifications were also introduced in Version 3, including improved mass consistency and diagnostic outputs. The CAMx version 3.01 is exercised for the September 1993 SuperCOAST ozone episode in this study including the application of the flexi-nesting features. Version 3.01 differs from version 3.0 only in a minor correction to the particle deposition algorithms, and does not impact the modeling performed in this study.

In August 2001, ENVIRON completed a study to examine and implement chlorine chemistry in version 3.01 of the CAMx model (ENVIRON, 2001). Recent evidence for the importance of chlorine within the Houston urban atmosphere comes from studies performed by the University of Texas at Austin (UT) as published by Tanaka, et al. (2000). The ENVIRON study successfully demonstrated the implementation of chlorine chemistry in the model and examined the impacts on ozone predictions in the Houston area.

The application of CAMx v3.01 using the modeling databases developed for the TNRCC SIP demonstration with CAMx version 2.03 presents some difficulties specifically related to the Plume-in-Grid (PiG) treatment in the different versions of the model. Likewise, the application of the flexi-nesting features poses additional concerns when utilizing the SIP databases. A significant modification in version 3.01 of CAMx is related to the internal consistency checks when the PiG algorithms are implemented. Prior to version 3.0, the CAMx model did not enforce the requirement that the ordering of PiG sources within the model ready emission files be internally consistent from day to day within the modeled episode. Thus, the version 2.03 model applications were able to simulate all days of the episode with the PiG algorithms. However, as the last day of the episode, September 11, 1993, includes point sources and PiG designations that differed from the preceding days, version 3.01 of the CAMx model will abort on this day. Although this last day is essentially a “clean-out” day, there are still relatively high levels of ozone within the Houston area, and it was therefore desirable to include this day for the current sensitivity simulations. Thus, the simulations presented and discussed in this report were performed with the PiG treatment disabled on September 11. While the ozone levels so obtained are still significant, and warrant evaluation, it must be noted that possibly a significant amount of NOx emissions are essentially lost when this day is started without PiG, having been stored within the NOx plumes due to the PiG application from previous simulation days. As the last day is run within the PiG treatment, there exists no mechanism for recovering this pollutant mass within the model.

Another factor to be considered is the use of the flexi-nesting features of version 3.01 in combination with PiG treatment. The PiG algorithms track NOx emissions within distinct plumes, the size and age of which are related to the model grid cell resolution. When the high resolution flexi-nest is introduced, existing PiGs within the simulation are exposed to a finer modeling grid which cause the pollutant mass to "dump" into the grid, thus affecting the model predicted ozone concentrations within the high resolution nested grid. These impacts would be minimized if the nest were introduced earlier in the simulation. In order to maximize computational resources, it was desirable to run the model without the high resolution nest during the "spin-up" period, September 6-8, 1993, introducing the nest on 8 September.

To assess the impact due to the introduction of the nest on predicted ozone levels during the episode days, two sensitivity simulations were performed.– one in which the nest was introduced at midnight on the 6th and one in which the nest was introduced at midnight on the 7th. The impacts on hourly simulated ozone concentrations where then compared and evaluated. Figure 2.5 displays these impacts at midnight and 10 am on September 8, 1993. As seen in Figure 2-5a, which displays the difference in predicted ozone between the two test simulations, the effect of introducing the nest the 8th rather than the 7th can be seen as localized increases and decreases in predicted ozone within and downwind of the high resolution grid. By 10 am on the 8th, these impacts are essentially negligible, as seen in Figure 2-5b. It was therefore determined that the model simulations, and particularly the predicted peaks and model performance on 8 September 1993, would not be significantly impacted due to these effects. All model simulation results with the flexi-nesting implementation presented in this report were obtained by introducing the nest on September 8, 1993, thereby minimizing the computational resource requirements.

As one of the overall objectives of the current study is to conduct VOC emission sensitivity simulations the importance of chemical interactions between NOx and VOC emissions is duly recognized. Because the PiG algorithms treat NOx emissions for PiG'd sources as distinct plumes, there would be no interaction with the VOC emissions for those sources treated with PiG. This raises concerns about the effectiveness, as well as the appropriateness of the VOC emission scenarios to be performed in later Tasks of the study. In addition, as all simulations performed thus far have used the Smolarkiewicz advection solver, which is known to be highly diffusive, it was felt that this last sensitivity simulation would be of more value overall if a more accurate up-to-date advection solver were used. Depending on the resulting model performance, this final model configuration may prove to be the most appropriate for conducting the emission sensitivity scenarios for the remainder of the study.

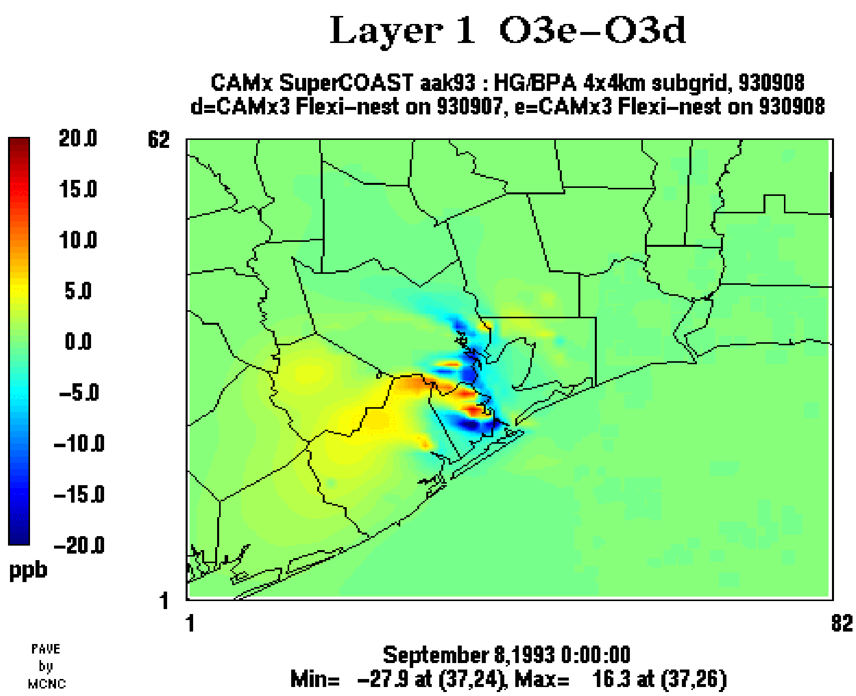

Figure 2-5a. Impacts of flexi-nest introduction on modeled ozone at midnight 8 September 1993.

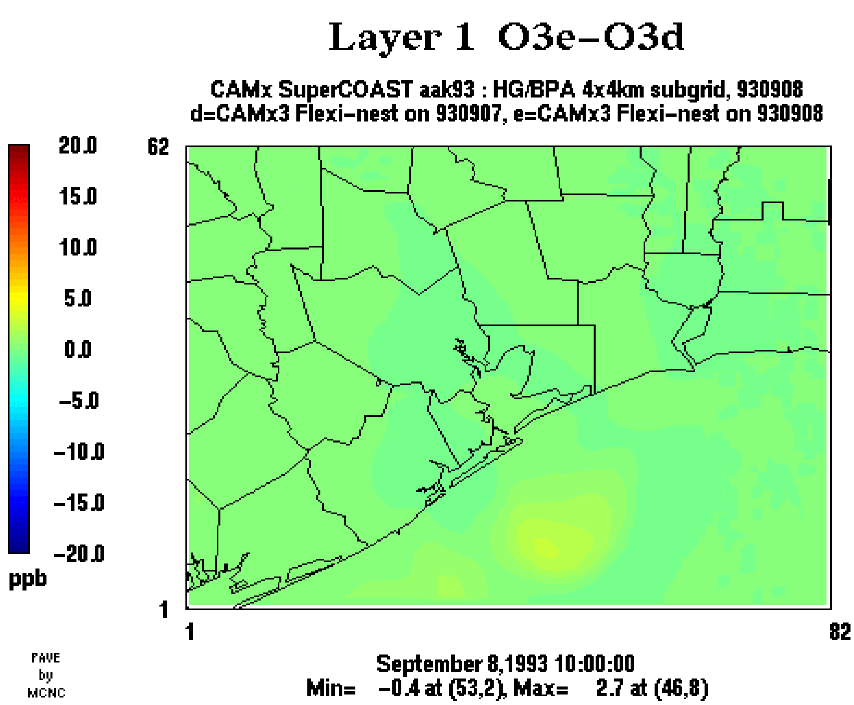

Figure 2-5b. Impacts of flexi-nest introduction on modeled ozone at 10 am on 8 September 1993.

3. MODELING RESULTS AND MODEL PERFORMANCE EVALUATION

Ozone modeling was performed for the Houston area (SuperCOAST domain) using CAMx version 2.03 and CAMx version 3.01, as described in section 2. The modeling used existing databases prepared by the TNRCC for the 8-11 September 1993 ozone episode in order to investigate model performance resulting from the implementation of various new features of the CAMx model. Version 2.03 of CAMx was applied primarily to establish a baseline simulation for comparison as well as to verify that the databases and model version used could reproduce the results obtained for the TNRCC SIP revision of December 2000.

As discussed above in Section 2, version of CAMx was applied both with and without chlorine emissions. In addition, the flexi-nesting capabilities available in CAMx version 3.01 were exercised on a 1.33-km grid encompassing the Houston Ship Channel and Galveston Bay. The flexi-nest was run both with and without chlorine emissions. The results of the simulation were evaluated with respect to EPA guidance on model performance evaluation.

The ozone modeling results for the September 1993 SuperCOAST domain episode are presented in a series of tables and figures in Appendices 3. Model spin-up days were generally excluded and so the results focus on September 8-11, 1993. The presentation of results also focuses on the 4-km grid area and, where applicable, the 1.33-km nested grid (Figure 2-2). The following results are presented:

- Tables of 1-hour ozone model performance statistics.
- Isopleth plots of daily maximum 1-hour ozone with observations for selected simulations.
- Isopleth plots of the difference in daily maximum 1-hour ozone due to different model versions and chlorine emissions.
- Time series of hourly 1-hour ozone observations and predictions.

Spatial Distribution of Daily Maximum 1-Hour Ozone

Figure 3-1 displays the spatial distribution of predicted daily maximum 1-hour ozone concentrations. As with all isopleth displays presented in this section, the figure consists of four separate panels, one for each episode day. In Figure 3-1, the results of the CAMx.v2.03 simulation in the 4-km HGBPA grid are shown for September 8-11, 1993. Also displayed are the observed daily maximum 1-hour ozone concentrations. The modeling results obtained using version 2.03 of CAMx are consistent with those obtained by the TNRCC, demonstrating the successful application of the code and databases. Figure 3-2 displays the corresponding results obtained with CAMx version 3.01. The overall spatial patterns of predicted ozone are similar with version 3.01 predicting slightly larger regions of elevated ozone concentrations. The predicted peaks are consistently higher throughout the episode and are slightly shifted in location with respect to the version 2.03 results. The increases in predicted peak ozone concentrations range from 20 to 33 ppb, depending on the episode day.

Figure 3-3 displays the spatial distributions of differences in predicted peak ozone concentrations between versions 3.01 and 2.03 of the CAMx model. The increased levels of ozone are generally confined to a small region. Relatively small changes are also evident throughout the domain on the order of 1 to 2 ppb.

The difference in ozone levels between CAMx versions 2.03 and 3.01 is attributed to improved algorithms in the vertical transport scheme. This difference is greater for the Houston simulations than other scenarios, presumably because of the high emission levels and pollutant concentrations in and around Houston.

The impact on predicted daily maximum ozone concentrations due to implementation of chlorine chemistry are displayed in Figure 3-4. Shown are isopleths of differences in daily maximum 1-hour ozone concentrations within the 4-km domain between CAMx version 3.01 simulations with and without chlorine emissions. The model predicts highly localized differences in peak ozone concentrations. The maximum differences occur close to the source of chlorine emissions with small differences (~1-2 ppb) extending downwind of the source. These results are consistent with the findings documented by ENVIRON as part of the study on the implementation of chlorine chemistry within the CAMx model (ENVIRON, 2001).

Results of the application of the flexi-nesting features of CAMX.v3.01 are displayed in Figure 3-5. Shown are isopleths of predicted daily maximum 1-hour ozone concentrations within the 1.33-km Houston grid. Also shown are the observed peak ozone data within the grid. Figure 3-6 displays the spatial distributions of differences in predicted daily maximum 1-hour ozone concentration within the 4-km HGBPA domain. The impact of the high resolution nested grid on predicted ozone levels are seen to be fairly localized decreases, occurring primarily in regions of elevated ozone levels within the industrial areas of the Houston region. Smaller ozone decreases are also evident. The increased grid resolution in the region of the Houston Ship Channel and Galveston Bay affords an improved treatment of point sources emissions, effectively resolving the spatial distribution of precursor emissions more accurately.

The modeling results obtained through application of both chlorine chemistry and the flexi-nesting features of version 3.01 of the CAMx model are displayed in Figure 3-7. Displayed are the differences in predicted daily maximum 1-hour ozone concentrations within the 1-33-km domain. As expected, the differences are generally seen to be highly localized increases in peak ozone levels confined to a region close to the sources of chlorine emissions. Much smaller increases are also evident downwind from the peak differences.

Figure 3-8 presents the results of the CAMx simulation using version 3.01 with the Piecewise Parabolic Method (PPM) advection scheme with flexi-nesting and without the PiG treatment of elevated point sources. Isopleths of daily maximum 1-hour ozone concentrations in the 4-km HGBPA domain are displayed. The spatial distribution of daily maximum ozone is similar to that obtained with the Smolarkiewicz advection scheme and with the PiG treatment, although the ozone peaks are somewhat higher on some episode days.

Model Performance Statistical Measures

The U.S. EPA has defined various statistical model performance measures in order to evaluate the results of air quality modeling performed in support of SIP development. These measures provide an indication of the model's ability to adequately reproduce observed pollutant concentrations. Performance goals are defined for the following statistics: accuracy of unpaired peak; mean normalized bias; and mean normalized gross error. Tables 3–1 through 3-3 present these performance measures for each of the sensitivity simulations performed as part of this study. The results for each simulation within the 4-km HGBPA domain are displayed in Table 3-1 for the September 8-11, 1993 episode days. As can be seen, all simulations result in acceptable performance with respect to EPA guidance. Depending on the episode day, the statistics may be better or worse for each simulation. The CAMx version 3.01 simulations with and without chlorine chemistry result in approximately equivalent model performance, while the simulation with both chlorine chemistry and flexi-nested is generally better, overall, than the results with version 3.01 with chlorine. The statistics presented appear to show the CAMx version 2.03 produces slightly better overall performance, however we do not attach much weight to this finding because of the reasons explained below.

Given the uncertainties and biases believed to exist in key model inputs, such as the SAIMM meteorology and the industrial emissions, we conclude that model performance is similar for all of the model configurations evaluated here and that the model configuration for use in further studies should be selected based on the best science.

Table 3-2 presents the statistical performance measures resulting from the application of flexi-nesting capabilities of CAMx version 3.01. Shown are the results of the simulations analyzed on the 4-km HGBPA domain with the PiG treatment and the Smolarkiewicz advection as well as the results of the simulation using the PPM advection scheme without PiG treatment. The statistics shown here were developed in such a way as to reflect the modeled concentrations at the appropriate modeled resolution. In other words, statistics within the 1.33-km domain sub-region of the 4-km domain are calculated using modeled results at 1.33-km while those outside the Houston fine grid domain are calculated using modeled concentrations at 4-km resolution. It is worthwhile to note that the observed peak ozone concentrations occur within the 1.33-km Houston domain for all episode days (September 8-11, 1993). As shown, the model performance is acceptable with respect to EPA guidance and, in some cases, is considerably better than the other simulations evaluated.

Time Series Plots

For completeness, time series plots for each of the simulations performed are presented in Figure 3-9 through Figure 3-11. The effects of changing the version of the model (v2.03 and v3.01), the modeling domain configuration (with and without flexi-nesting) and the chemistry (with and without chlorine emissions) can be seen with respect to the temporal variation of the predicted hourly ozone concentrations. The ability of the model to replicate the observed hourly ozone concentrations at the monitoring sites is illustrated and is reflected in the overall statistical performance measures presented in Tables 3-1 and 3-2.

Table 3-1. CAMx Model Evaluation Statistics for the 8-11 September 1993 Episode on 4-km HGBPA Domain.

Performance Attribute	EPA Goal	8 Sept	9 Sept	10 Sept	11 Sept
Maximum Observed Concentration (ppb)		214.0	195.0	162.0	189.0
Maximum Modeled Conc. (ppb)					
CAMx v2.03		186.9	174.7	172.1	181.6
CAMx v3.01		195.1	183.4	180.5	186.9
CAMx v3.01 w/ Cl		195.7	183.9	181.6	187.5
CAMx v3.01 w/ Flexi-nest		196.3	189.5	179.9	187.4
CAMx v3.01 w/ Flexi-nest and Cl		196.8	189.9	180.9	188.1
Accuracy of Unpaired Peak (%)	< "20%				
CAMx v2.03		-12.7	-10.4	6.2	-3.9
CAMx v3.01		-8.9	-5.9	11.4	-1.1
CAMx v3.01 w/ Cl		-8.6	-5.7	12.1	-0.8
CAMx v3.01 w/ Flexi-nest		-8.3	-2.8	11.0	-0.9
CAMx v3.01 w/ Flexi-nest and Cl		-8.1	-2.6	11.7	-0.5
Mean Normalized Bias (%)	< "15%				
CAMx v2.03		5.0	3.1	-9.4	1.0
CAMx v3.01		9.9	8.21	-5.5	4.8
CAMx v3.01 w/ Cl		10.7	8.7	-4.7	5.6
CAMx v3.01 w/ Flexi-nest		8.2	6.6	-7.2	2.8
CAMx v3.01 w/ Flexi-nest and Cl		9.0	7.1	-6.5	3.7
Mean Normalized Gross Error (%)	< "35%				
CAMx v2.03		21.8	23.6	23.6	18.8
CAMx v3.01		24.0	26.2	24.9	19.9
CAMx v3.01 w/ Cl		24.3	26.4	25.1	20.1
CAMx v3.01 w/ Flexi-nest		23.9	25.7	24.4	20.1
CAMx v3.01 w/ Flexi-nest and Cl		24.2	25.9	24.6	20.2

Table 3-2. CAMx Model Evaluation Statistics for the 8-11 September 1993 Episode at 1.33-km Resolution in the HGBPA 4-km Domain.

Performance Attribute	EPA Goal	8 Sept	9 Sept	10 Sept	11 Sept
Maximum Observed Concentration (ppb)		214.0	195.0	162.0	189.0
Maximum Modeled Conc. (ppb)					
CAMx v3.01 w/ Flexi-nest and Cl		196.8	192.4	180.9	188.1
CAMx v3.01 w/Flexi-nest and Cl – PPM advection solver w/o PiG		207.1	198.0	189.6	193.8
Accuracy of Unpaired Peak (%)	< "20%				
CAMx v3.01 w/ Flexi-nest and Cl		-8.1	-1.3	11.7	-0.5
CAMx v3.01 w/Flexi-nest and Cl – PPM advection solver w/o PiG		-3.2	1.5	17.1	2.5
Mean Normalized Bias (%)	< "15%				
CAMx v3.01 w/ Flexi-nest and Cl		8.4	6.9	-7.2	3.0
CAMx v3.01 w/Flexi-nest and Cl – PPM advection solver w/o PiG		7.1	5.3	-10.1	0.7
Mean Normalized Gross Error (%)	< "35%				
CAMx v3.01 w/ Flexi-nest and Cl		25.0	26.9	25.4	20.7
CAMx v3.01 w/Flexi-nest and Cl – PPM advection solver w/o PiG		25.4	27.4	25.7	21.4

4. SUMMARY

The CAMx air quality model was applied to the September 8-11, 1993 ozone episode on the SuperCOAST domain. Versions 2.03 and 3.01 were implemented and the results reviewed with respect to EPA guidance on model performance. New features of CAMx including the addition of chlorine chemistry and the flexi-nesting capabilities were applied and evaluated. The purpose of the various sensitivity simulations was primarily to determine the most appropriate model version and configuration to be used for conducting further emission sensitivity analyses on the SuperCOAST modeling domain for the September 1993 ozone episode.

The modeling results documented here indicate that version 3.01 of the CAMx model is capable of successfully simulating the observed concentrations of ozone occurring in the Houston urban area during the episode. In addition, the new features of version 3.01 – chlorine chemistry and flexi-nesting- were successfully applied for the episode and result in acceptable model performance with respect to EPA guidance on air quality model evaluation for SIP development.

The following conclusions can be drawn from the model simulations evaluated here:

- All model configurations evaluated result in acceptable model performance with respect to EPA guidance. Statistical measures of peak accuracy, normalized bias and normalized gross error all meet the goals set forth by the EPA for SIP modeling demonstrations.

- Based on the differences in modeled concentrations of daily maximum 1-hour ozone in the Houston urban area and more generally within the SuperCOAST modeling domain, the application of version 3.01 of CAMx would not significantly change the response to emissions scenarios used by the TNRCC for control strategy evaluation.

- Given the uncertainties and biases believed to exist in key model inputs, such as the SAIMM meteorology and the industrial emissions, we conclude that model performance is similar for all of the model configurations evaluated here and that the model configuration for use in further studies should be selected based on the best science.

Based on the results of the model evaluations performed under this task, it is recommended to use version 3.01 of the CAMx model for further emission sensitivity simulations. The model configuration should make use of the updated chlorine chemistry and include the 1.33-km Houston nested grid domain. In order to adequately simulate the interaction of NOx and VOC emission within the industrial area within and around the Houston Ship Channel and Galveston Bay, the Plume-in-Grid treatment of large NOx sources should not be implemented. Finally, the advection scheme used in the simulations should be the Piecewise Parabolic Method in order to minimize the overly diffusive effects seen with the Smolarkiewicz solver.

5. REFERENCES

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APPENDIX A

Ozone Isopleth Displays

Figure 3-1. Daily maximum ozone concentrations for September 8-11, 1993. CAMx version 2.03.

Figure 3-2. Daily maximum ozone concentations for September 8-11, 1993. CAMx version 3.01.

Figure 3-3. Differences in 1-hour daily maximum ozone concentrations for September 8-11, 1993. CAMx version 3.01 minus version 2.03.

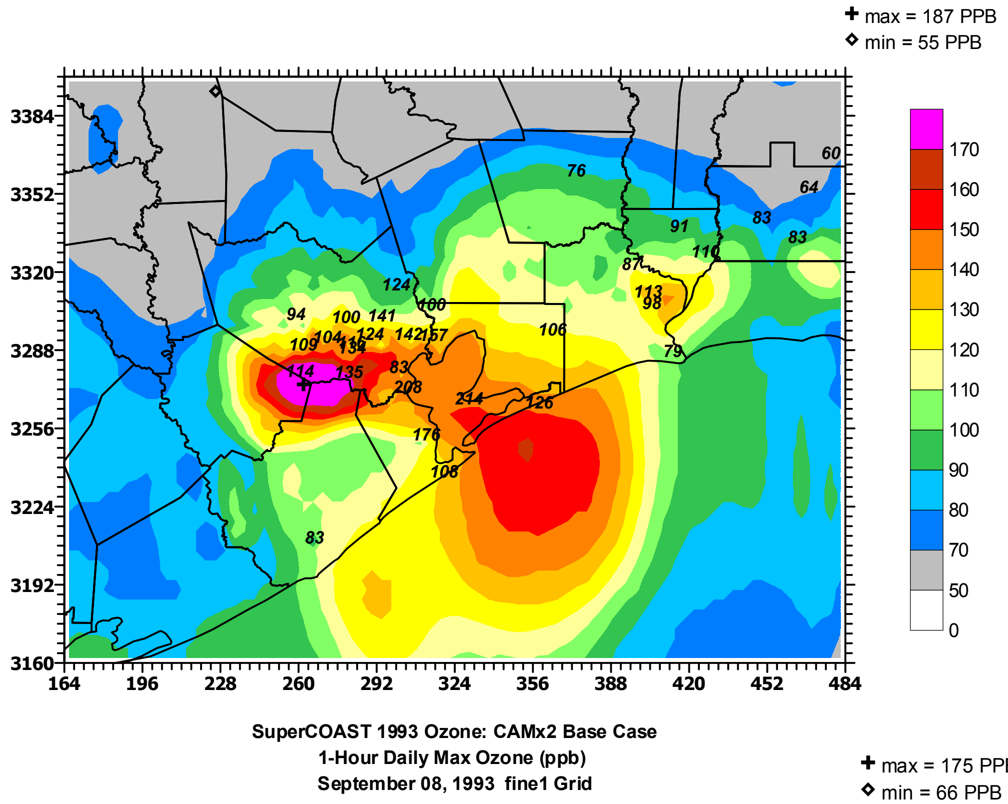
Figure 3-4. Daily maximum ozone concentrations for September 8-11, 1993 In 1.33-km flexi-nested grid.

Figure 3-5. Difference in 1-hour daily maximum ozone concentrations in Sept. 8-11, 1993. CAMx version 3.01 with and without 1.33-km flexi-nested grid.

Figure 3-6. Difference in 1-hour daily maximum ozone concentrations on September 8-11, 1993. CAMx version 3.01 with and without chlorine emissions.

Figure 3-7. Differences in 1-hour daily maximum ozone concentrations on Sept. 8-11, 1993 in the 1.33-km grid. CAMx version 3.01 with and without chlorine.

Figure 3-8. Daily maximum ozone concentrations for September 8-11, 1993. CAMx version 3.01 with PPM advection scheme and no PiG.



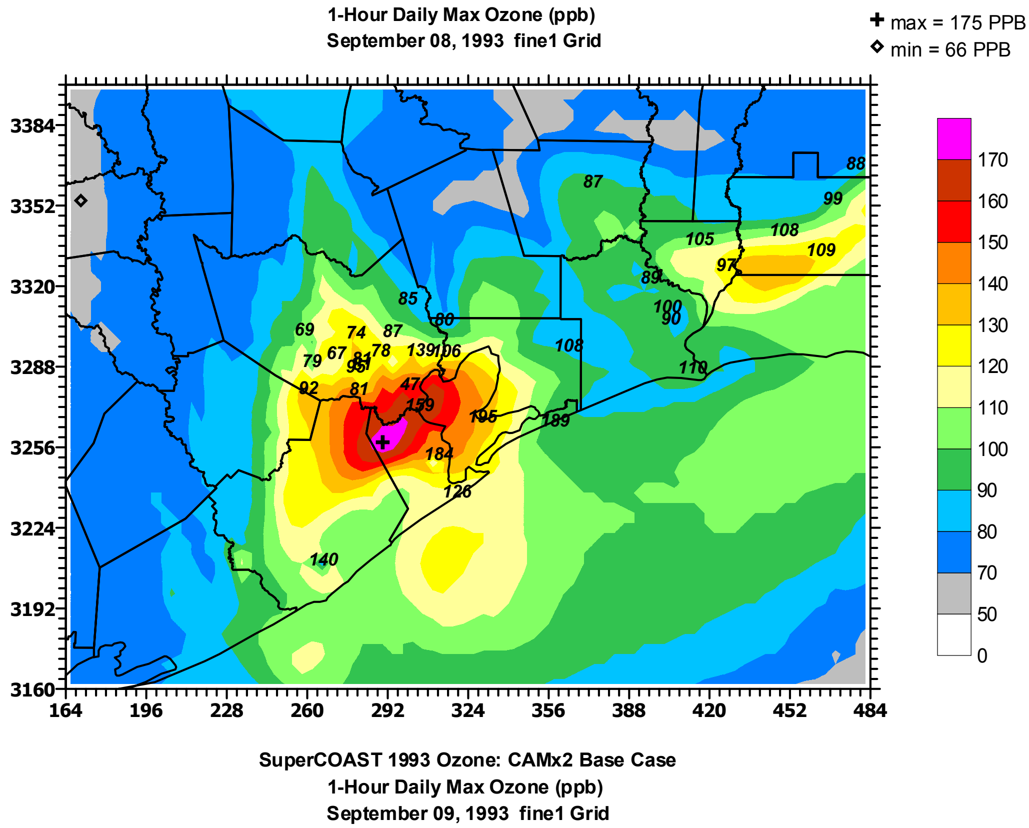
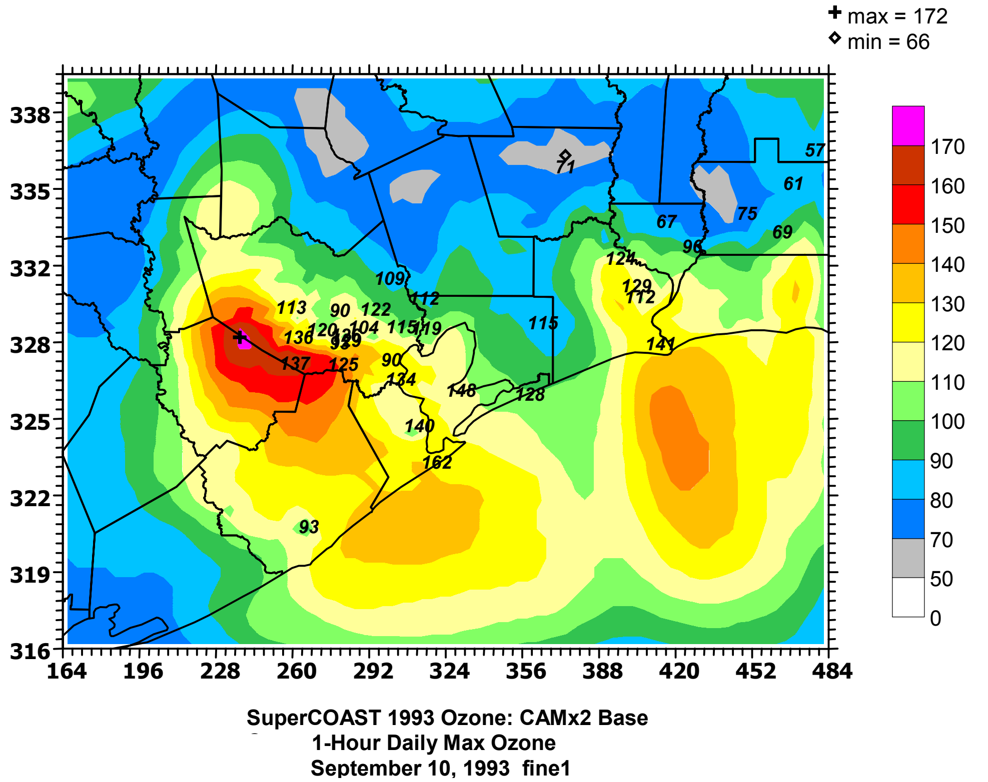


Figure 3-1. Daily maximum ozone concentrations for September 8-11, 1993. CAMx version 2.03.



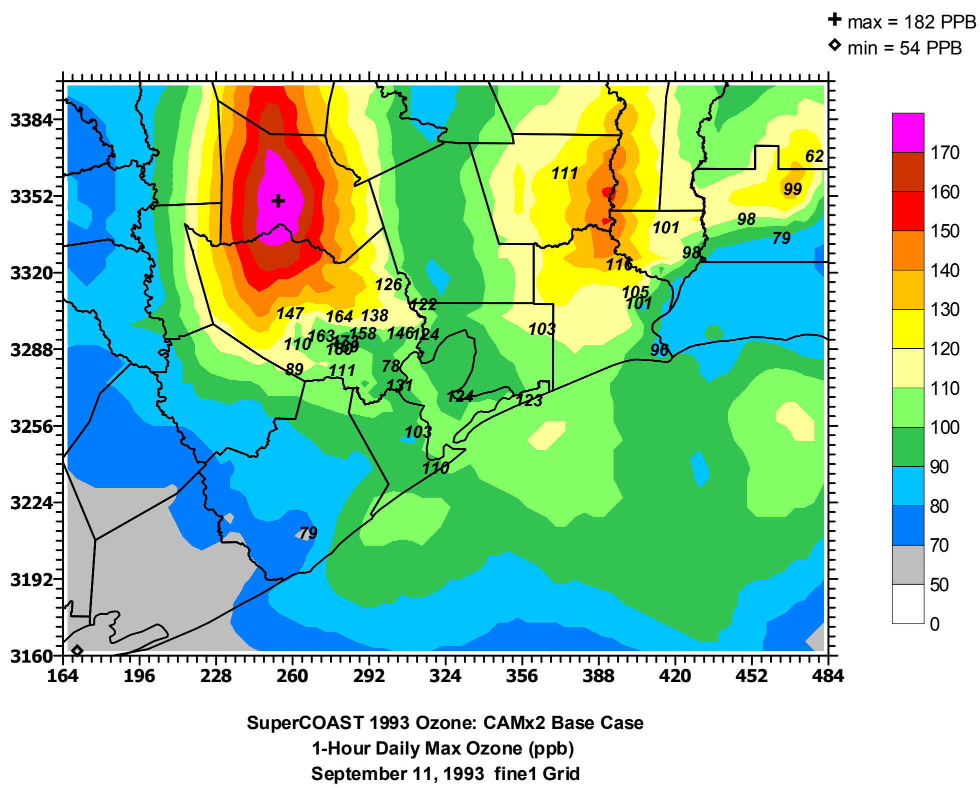
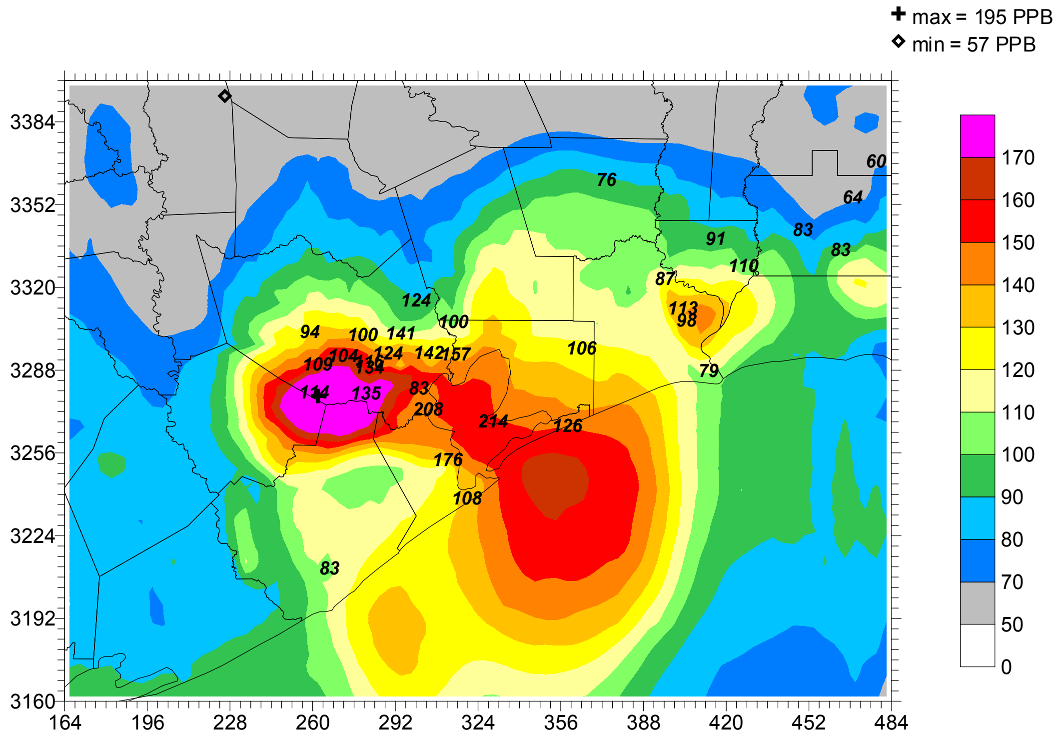
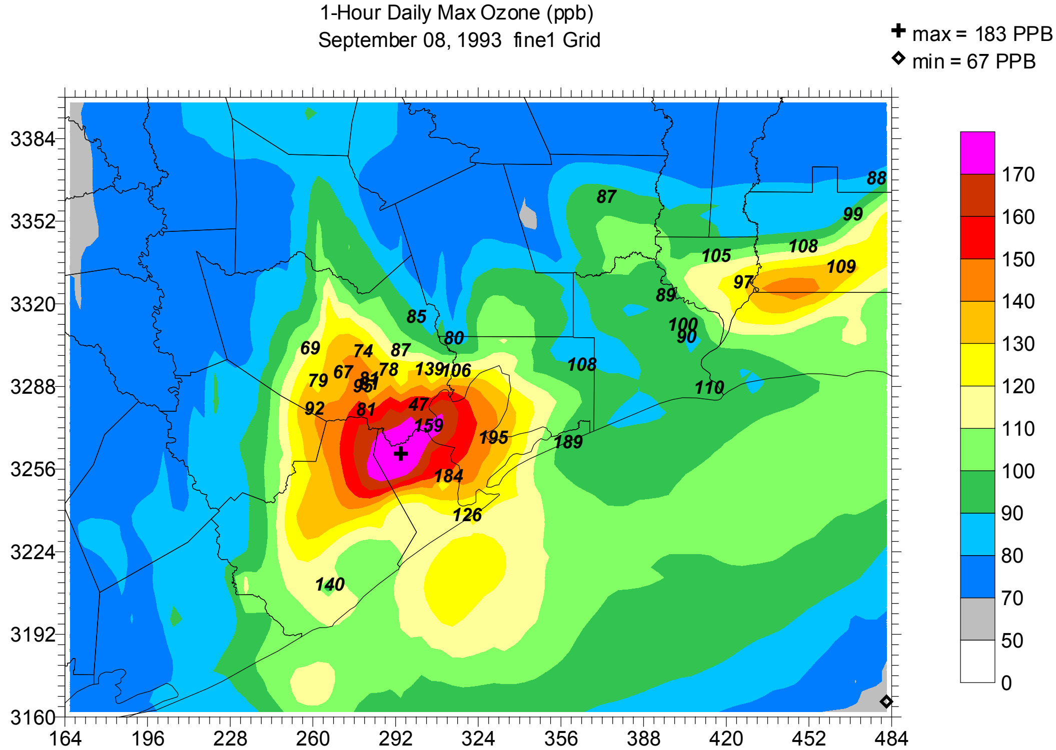


Figure 3-1 (continued). Daily maximum ozone concentrations for September 8-11, 1993 CAMx version 2.03.

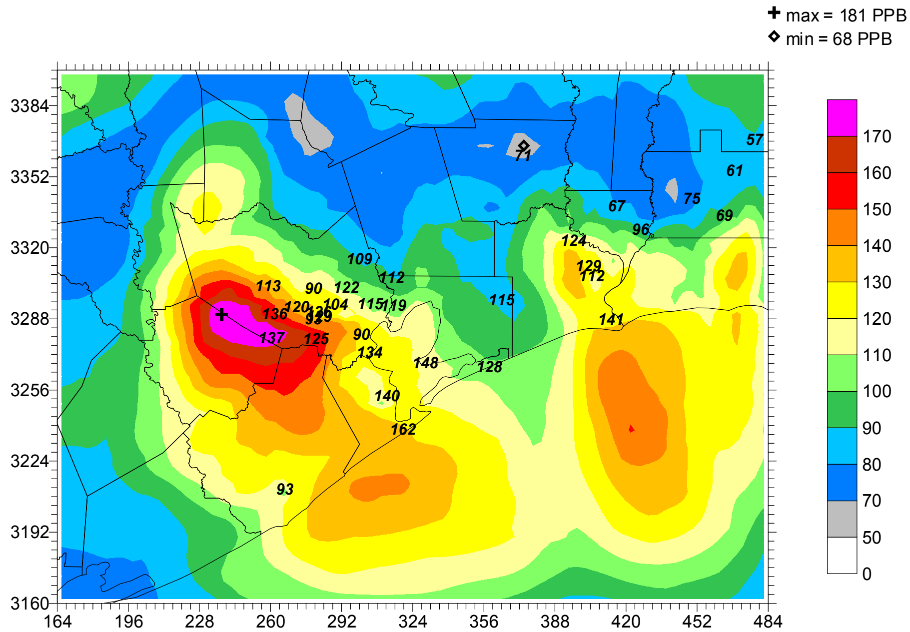


SuperCOAST 1993 Ozone: CAMx3 Base Case
1-Hour Daily Max Ozone (ppb)
September 08, 1993 fine1 Grid

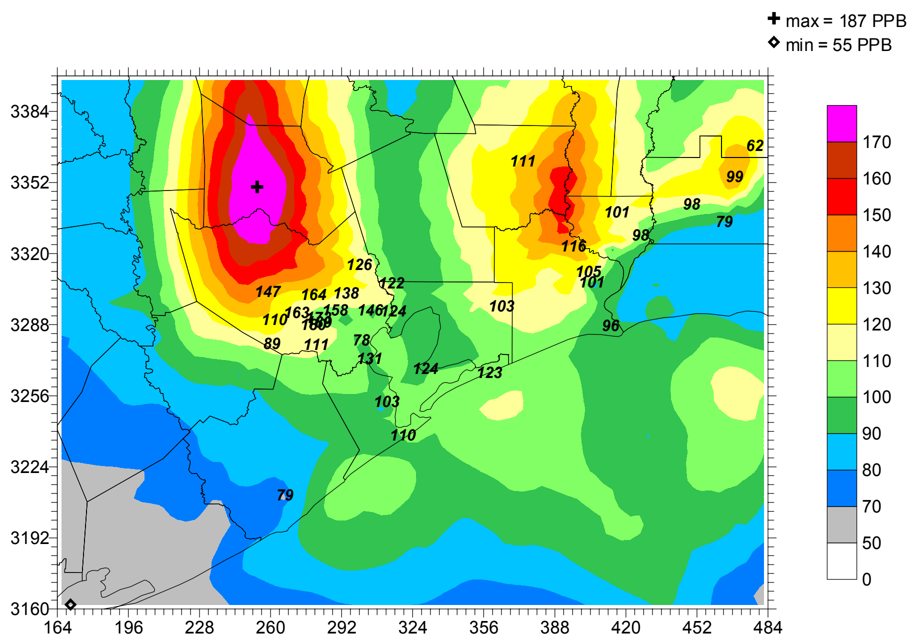


SuperCOAST 1993 Ozone: CAMx3 Base Case
1-Hour Daily Max Ozone (ppb)
September 09, 1993 fine1 Grid

Figure 3-2. Daily maximum ozone concentrations for September 8-11, 1993 CAMx version 3.01.

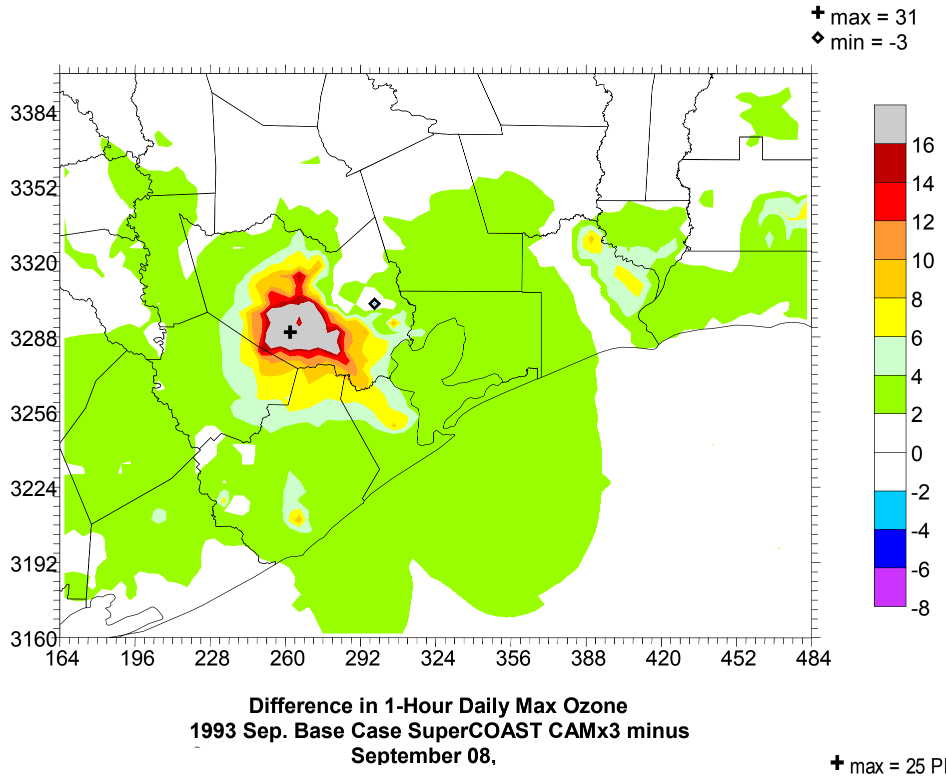


SuperCOAST 1993 Ozone: CAMx3 Base Case
1-Hour Daily Max Ozone (ppb)
September 10, 1993 fine1 Grid



SuperCOAST 1993 Ozone: CAMx3 Base Case
1-Hour Daily Max Ozone (ppb)
September 11, 1993 fine1 Grid

Figure 3-2 (continued). Daily maximum ozone concentrations for September 8-11, 1993 CAMx version 3.01.



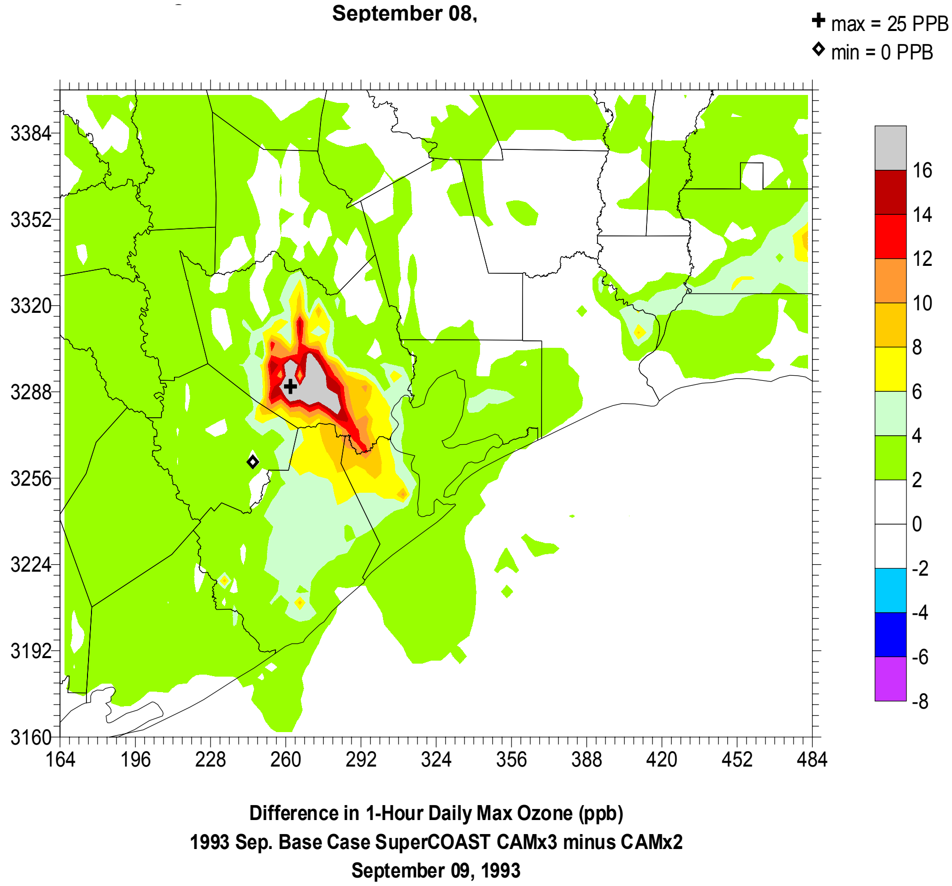
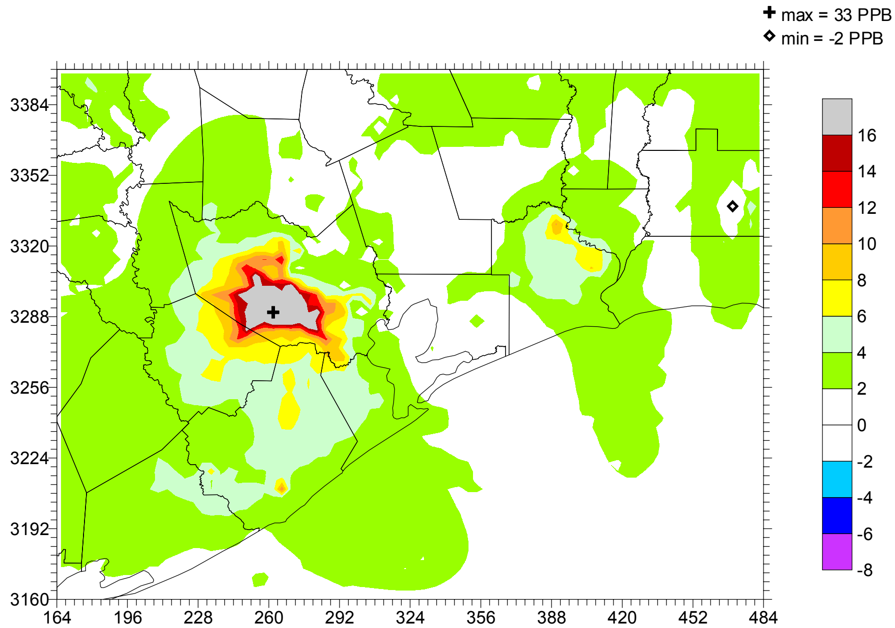
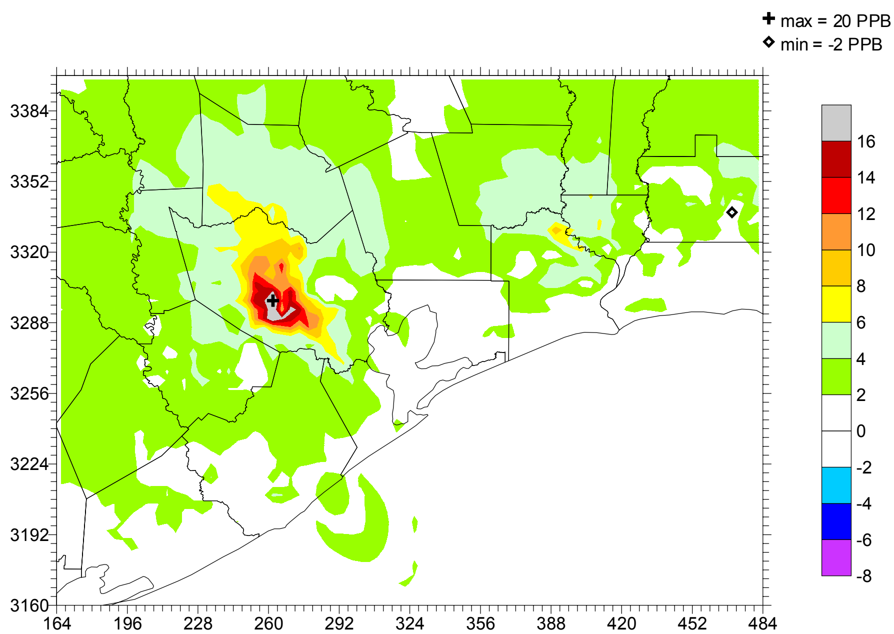


Figure 3-3. Differences in 1-hour daily maximum ozone concentrations for September 8-11, 1993. CAMx version 3.01 minus version 2.03.



Difference in 1-Hour Daily Max Ozone (ppb)
1993 Sep. Base Case SuperCOAST CAMx3 minus CAMx2
September 10, 1993



Difference in 1-Hour Daily Max Ozone (ppb)
1993 Sep. Base Case SuperCOAST CAMx3 minus CAMx2
September 11, 1993

Figure 3-3 (continued) Differences in 1-hour daily maximum ozone concentrations for September 8-11, 1993. CAMx version 3.01 minus CAMx version 2.03.

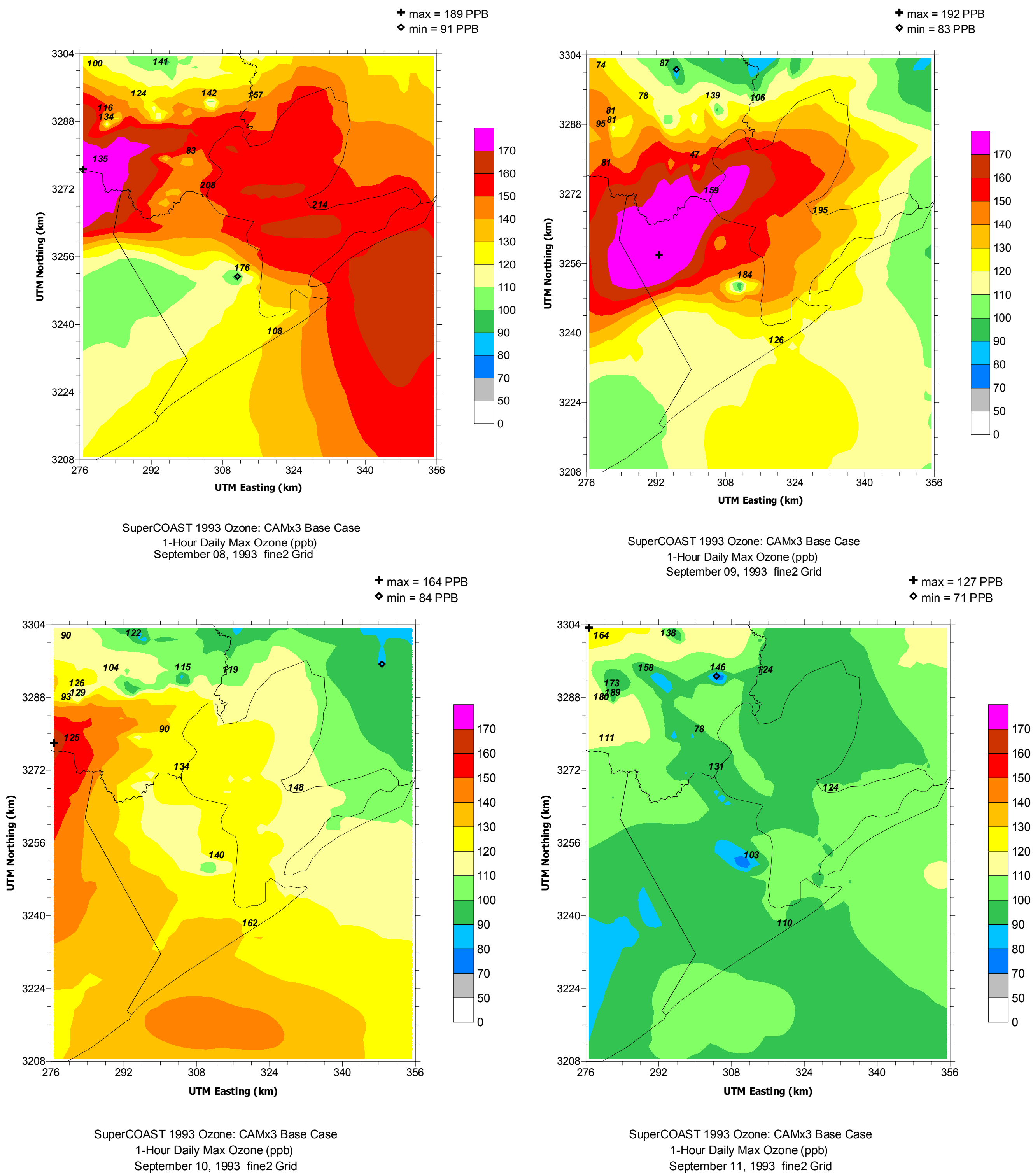


Figure 3-4. Daily maximum ozone concentrations for Sept. 8-11, 1993 in 1.33-km flexi-nested grid.

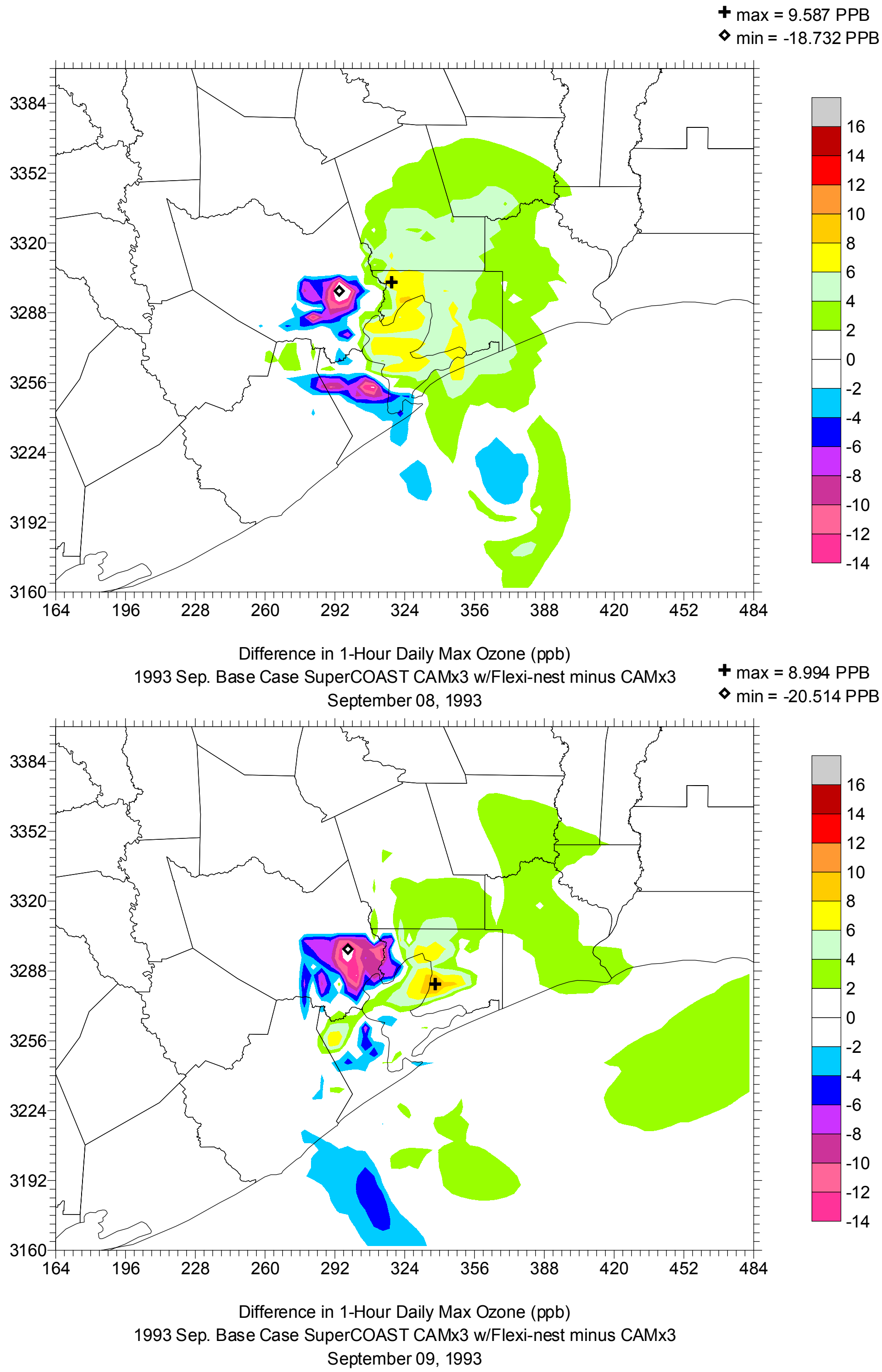
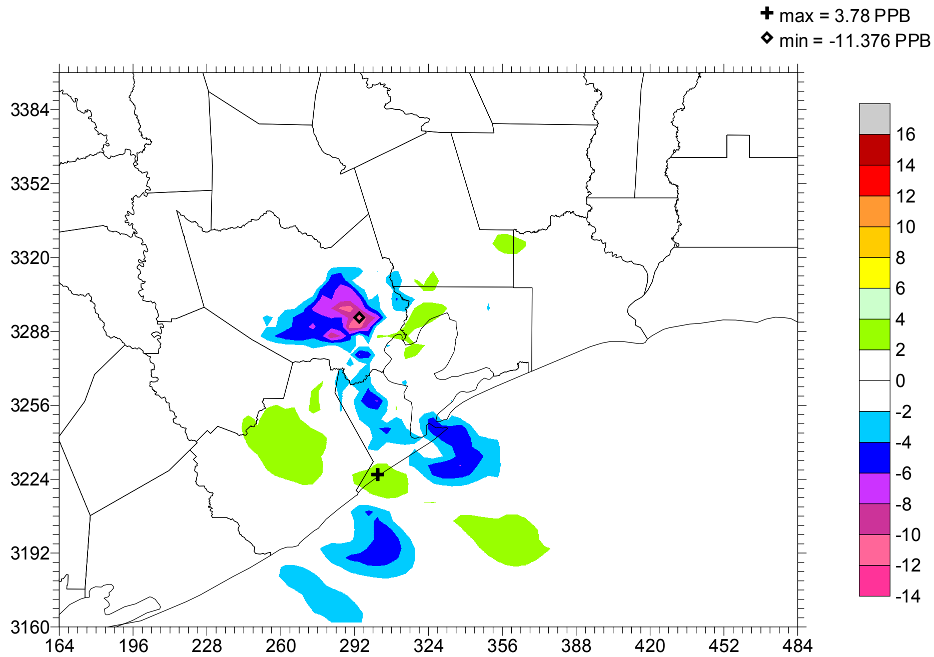
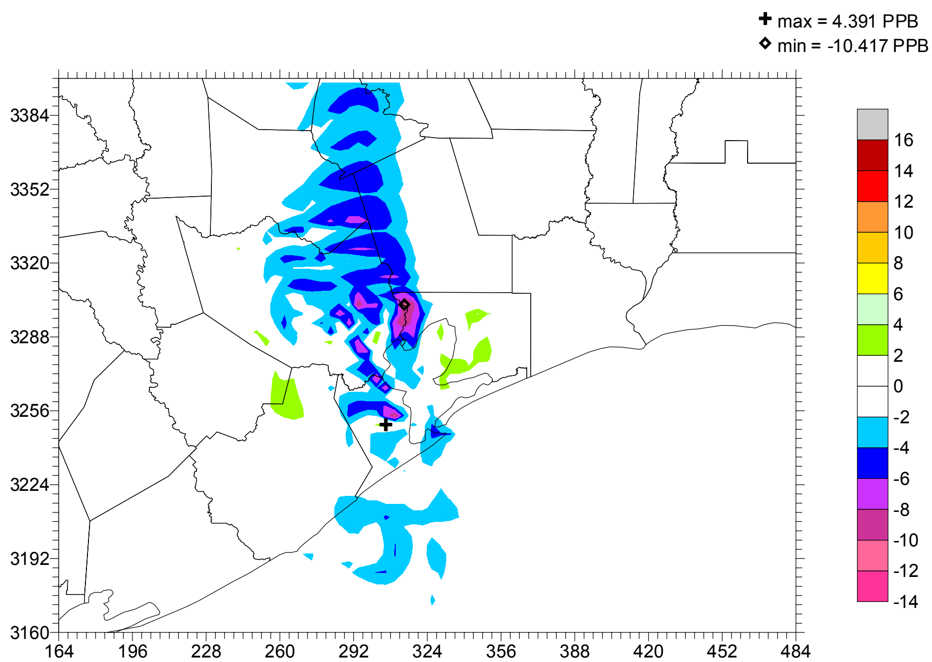


Figure 3-5. Difference in 1-hour daily maximum ozone concentrations in Sept. 8-11, 1993. CAMx.version 3.01 with and without 1.33-km flexi-nested grid.

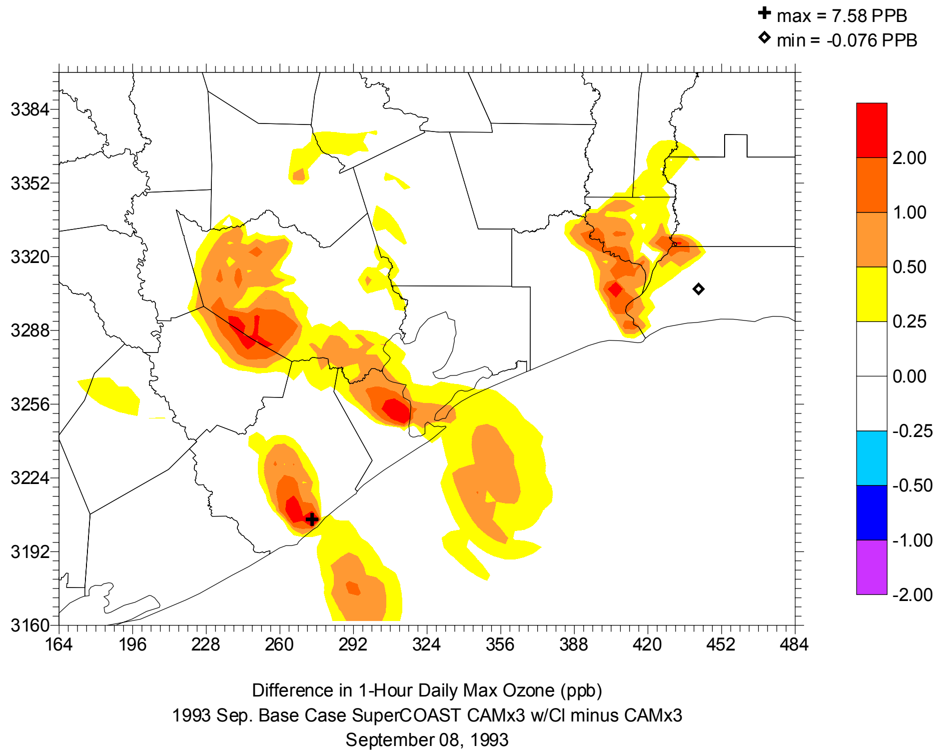


Difference in 1-Hour Daily Max Ozone (ppb)
1993 Sep. Base Case SuperCOAST CAMx3 w/Flexi-nest minus CAMx3
September 10, 1993



Difference in 1-Hour Daily Max Ozone (ppb)
1993 Sep. Base Case SuperCOAST CAMx3 w/Flexi-nest minus CAMx3
September 11, 1993

Figure 3-5 (continued). Difference in 1-hour daily maximum ozone concentrations in Sept. 8-11, 1993. CAMx version 3.01 with and without 1.33-km flexi-nested grid.



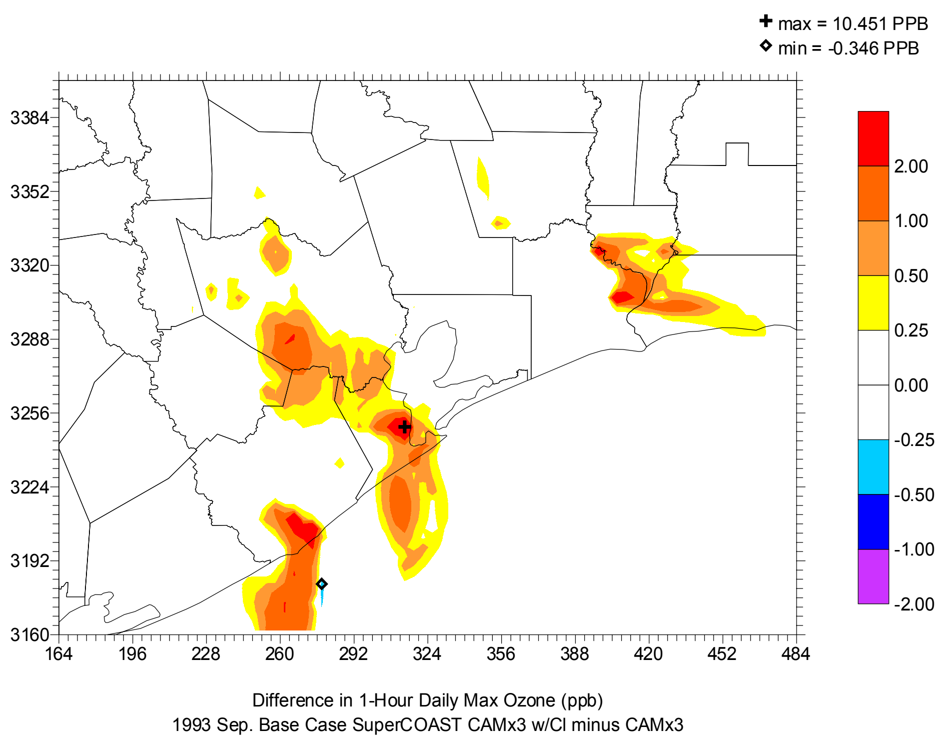
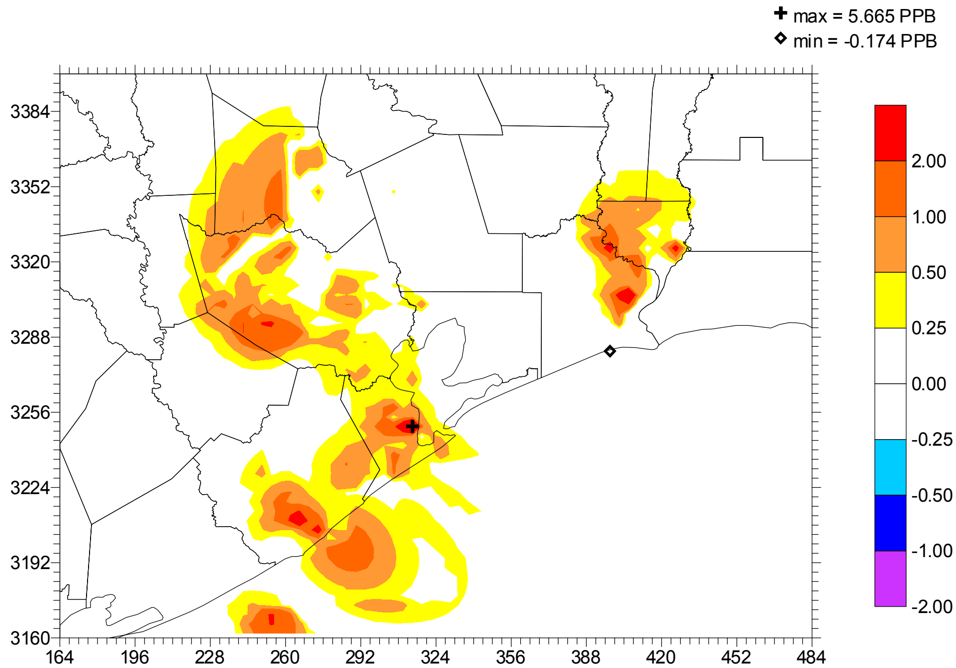
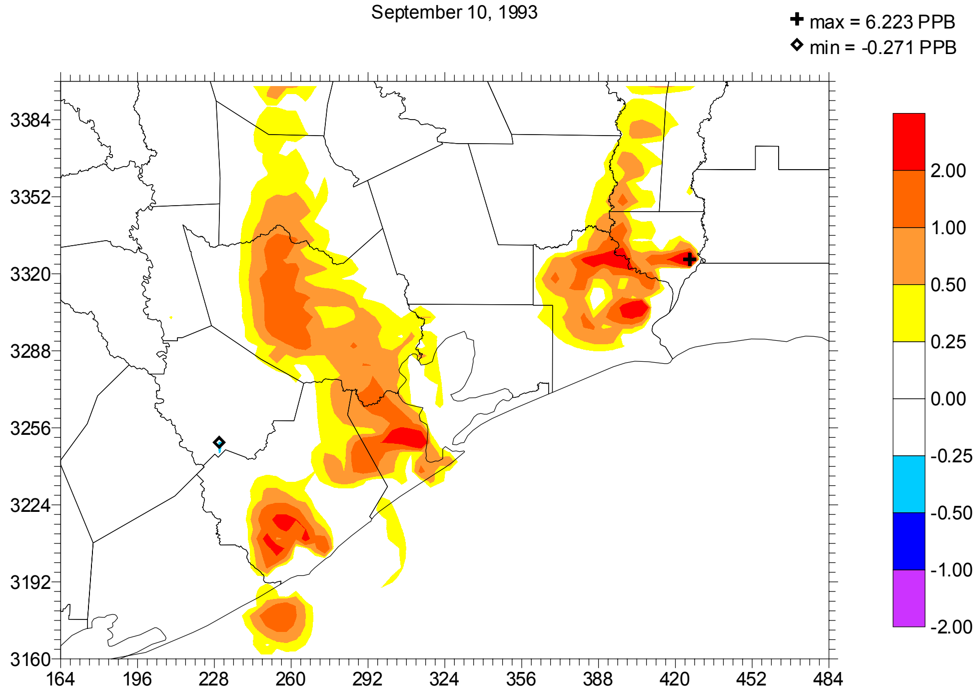


Figure 3-6. Difference in 1-hour daily maximum ozone concentrations on September 8-11, 1993. CAMx version 3.01 with and without chlorine emissions.



Difference in 1-Hour Daily Max Ozone (ppb)
1993 Sep. Base Case SuperCOAST CAMx3 w/Cl minus CAMx3
September 10, 1993



Difference in 1-Hour Daily Max Ozone (ppb)
1993 Sep. Base Case SuperCOAST CAMx3 w/Cl minus CAMx3
September 11, 1993

Figure 3-6 (continued). Difference in 1-hour daily maximum ozone concentrations on September 8-11, 1993. CAMx version 3.01 with and without chlorine emissions.

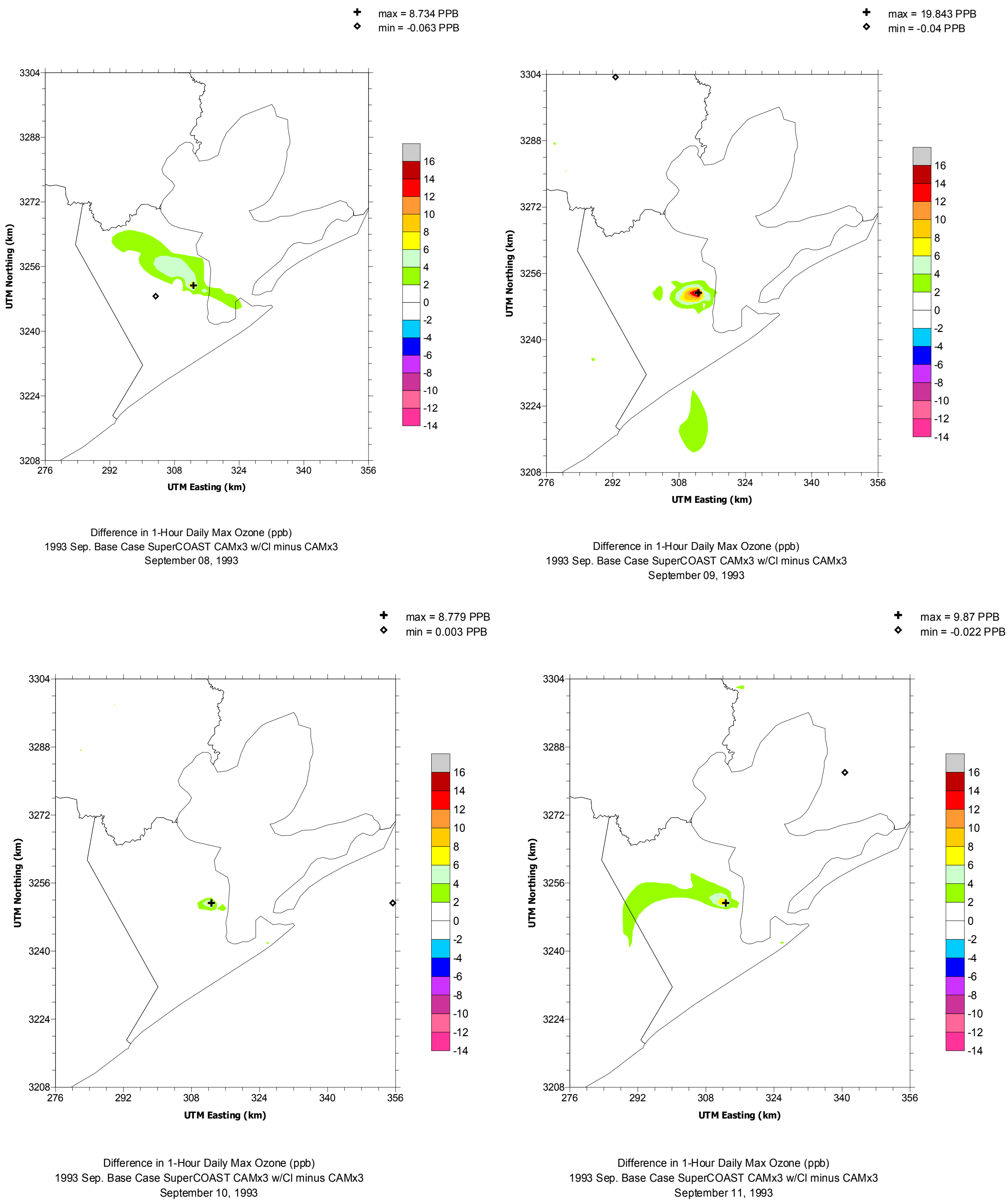
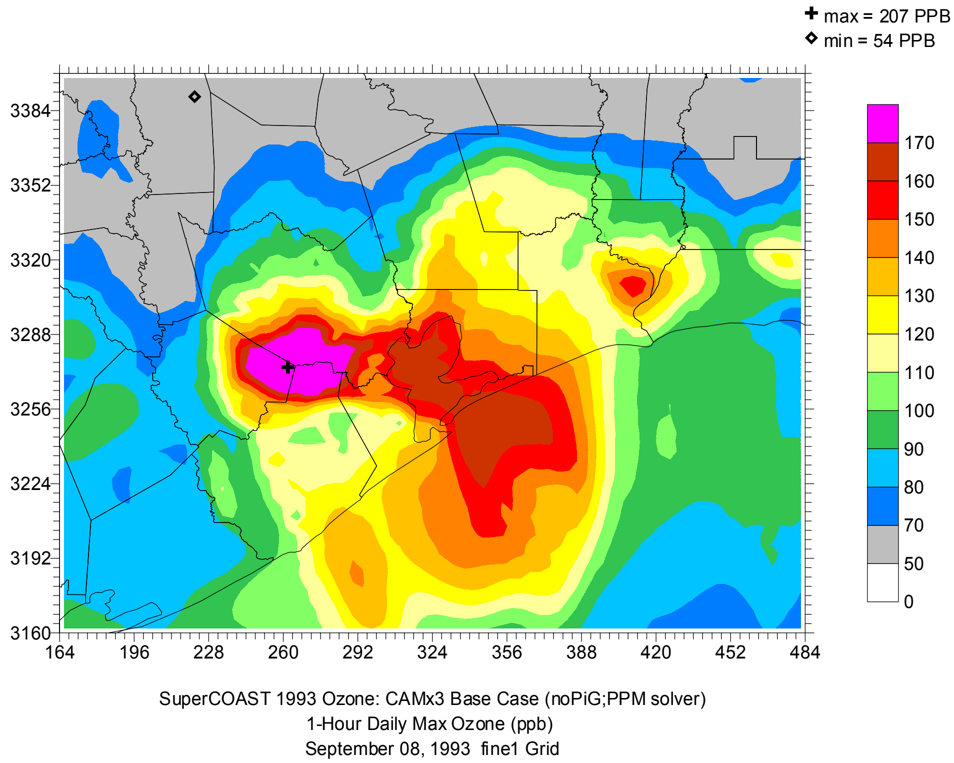


Figure 3-7. Differences in 1-hour daily maximum ozone concentrations on Sept. 8-11, 1993 in the 1.33-km grid. CAMx version 3.01 with and without chlorine.



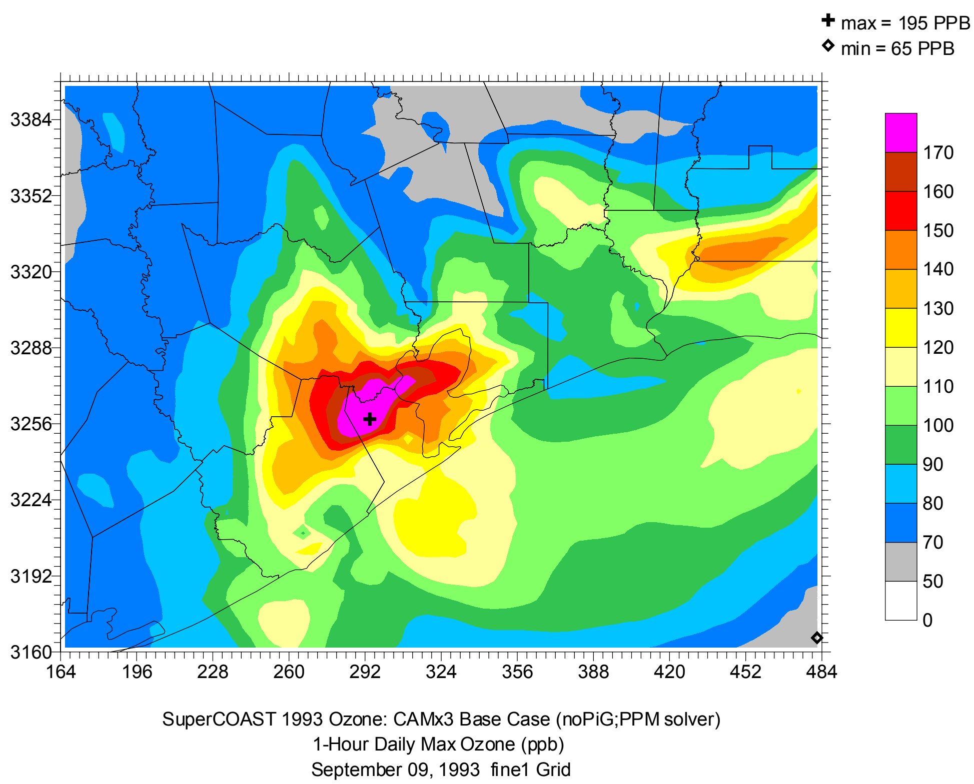
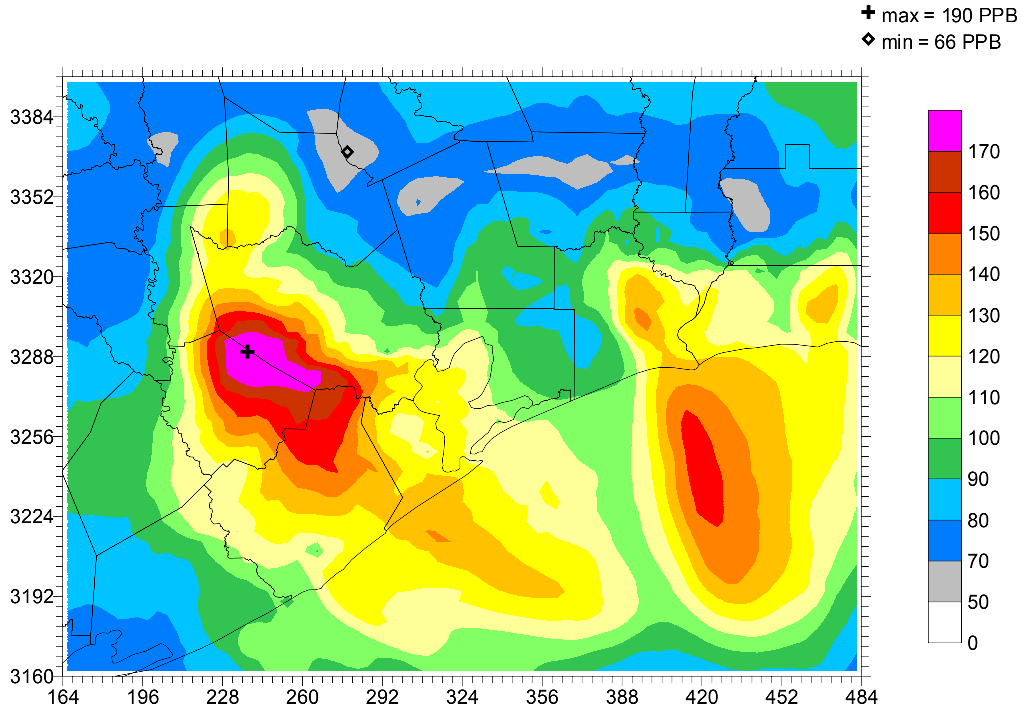
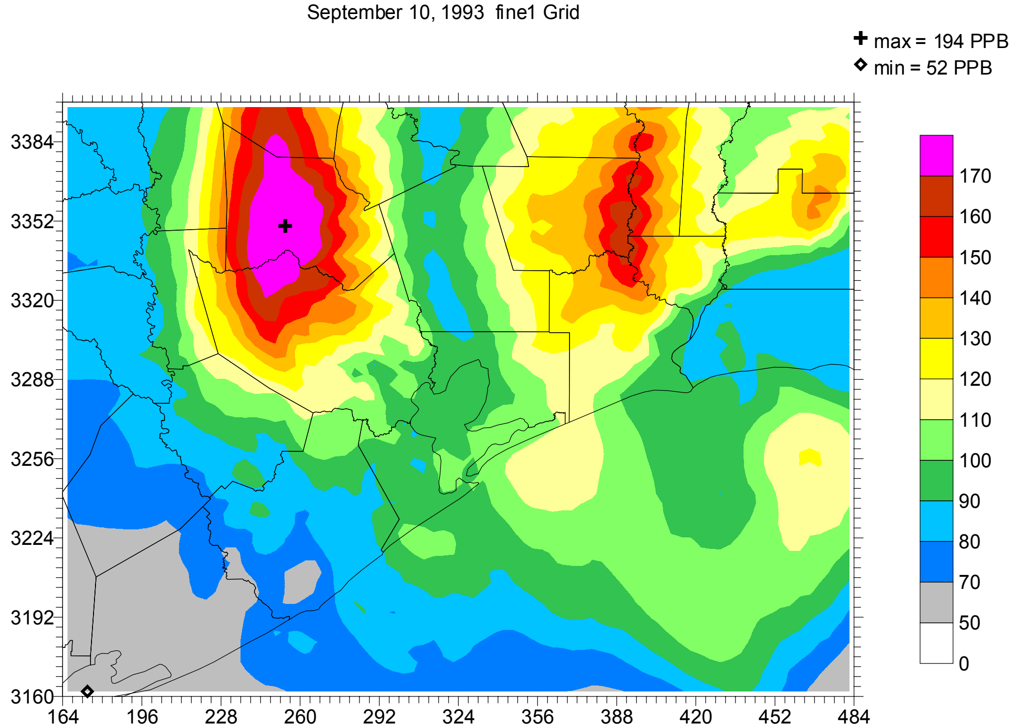


Figure 3-8. Daily maximum ozone concentrations for September 8-11, 1993. CAMx version 3.01 with PPM advection scheme and no PiG.



SuperCOAST 1993 Ozone: CAMx3 Base Case (noPiG;PPM solver)
1-Hour Daily Max Ozone (ppb)
September 10, 1993 fine1 Grid



SuperCOAST 1993 Ozone: CAMx3 Base Case (noPiG;PPM solver)
1-Hour Daily Max Ozone (ppb)
September 11, 1993 fine1 Grid

Figure 3.8 (continued). Daily maximum ozone concentrations for September 8-11, 1993. CAMx version 3.01 with PPM advection scheme and no PiG.

Appendix B

Plots

Figure 3-9. Time series of observed and predicted hourly ozone concentration within the 4-km HGBPA domain. CAMx versions 2.03 and 3.01

Figure 3-10. Time series of observed and predicted hourly ozone concentrations within the 4-km HGBPA domain. CAMx version 3.01 with and without chlorine emissions.

Figure 3-11. Time series of observed and predicted hourly ozone concentrations within the 4-km HGBPA domain. Results shown are calculated based on 1.33 km resolution CAMx version 3.01 with flexi-nest, PPM, and Smolarkiewicz advection schemes

SuperCOAST September 6-11,1993

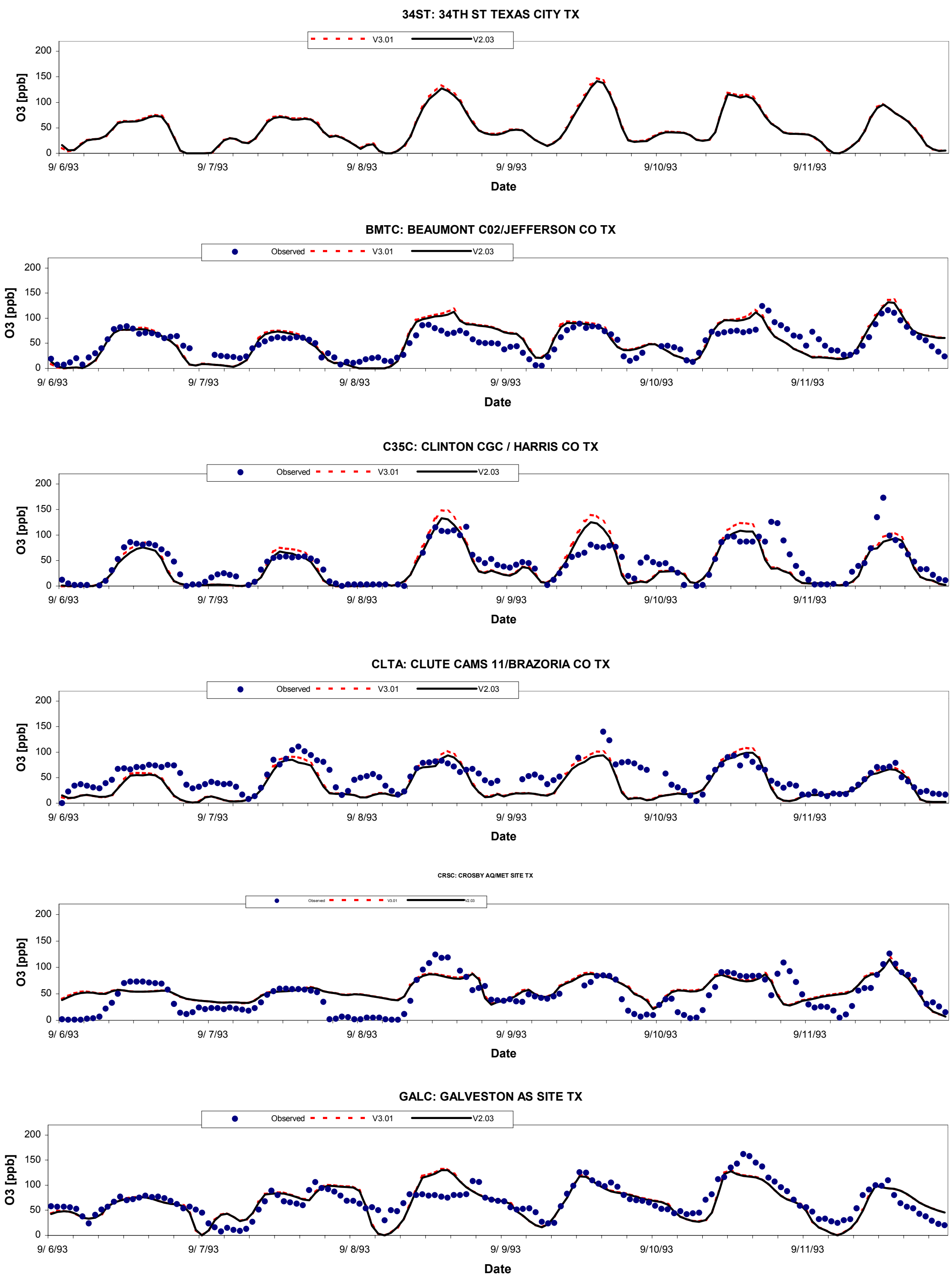


Figure 3-9.

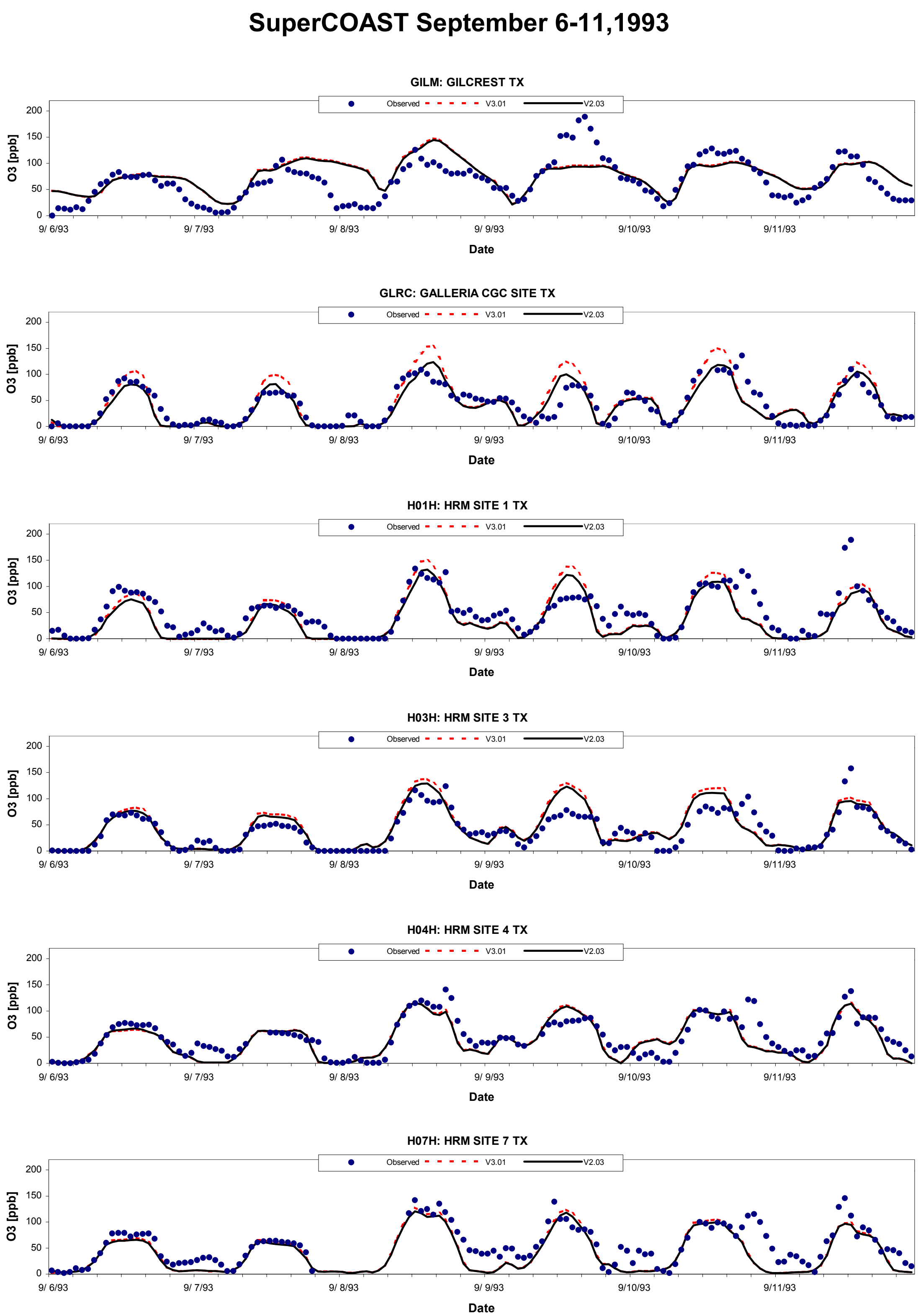


Figure 3-9. (continued).

SuperCOAST September 6-11,1993

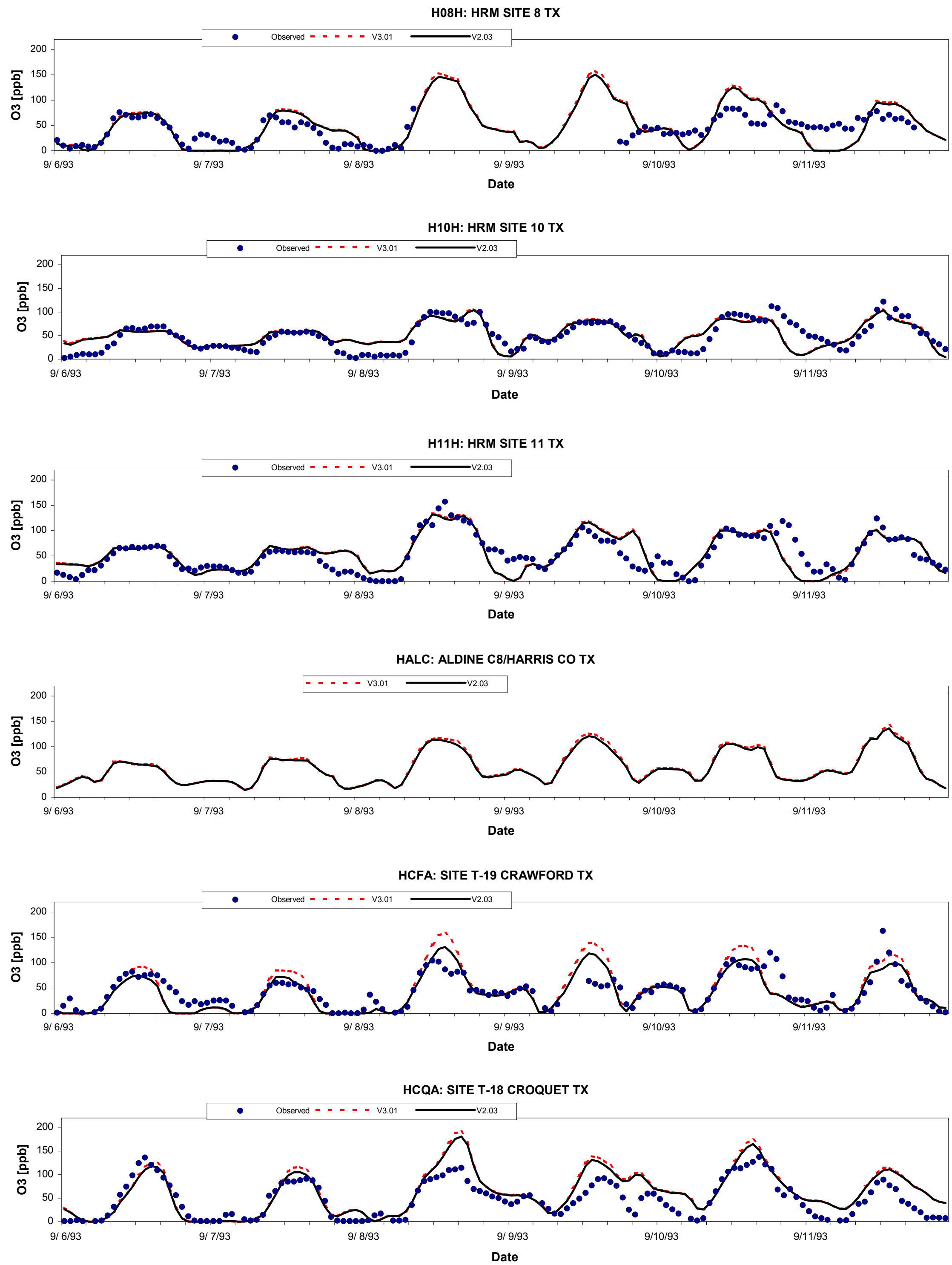


Figure 3-9. (continued).

SuperCOAST September 6-11,1993

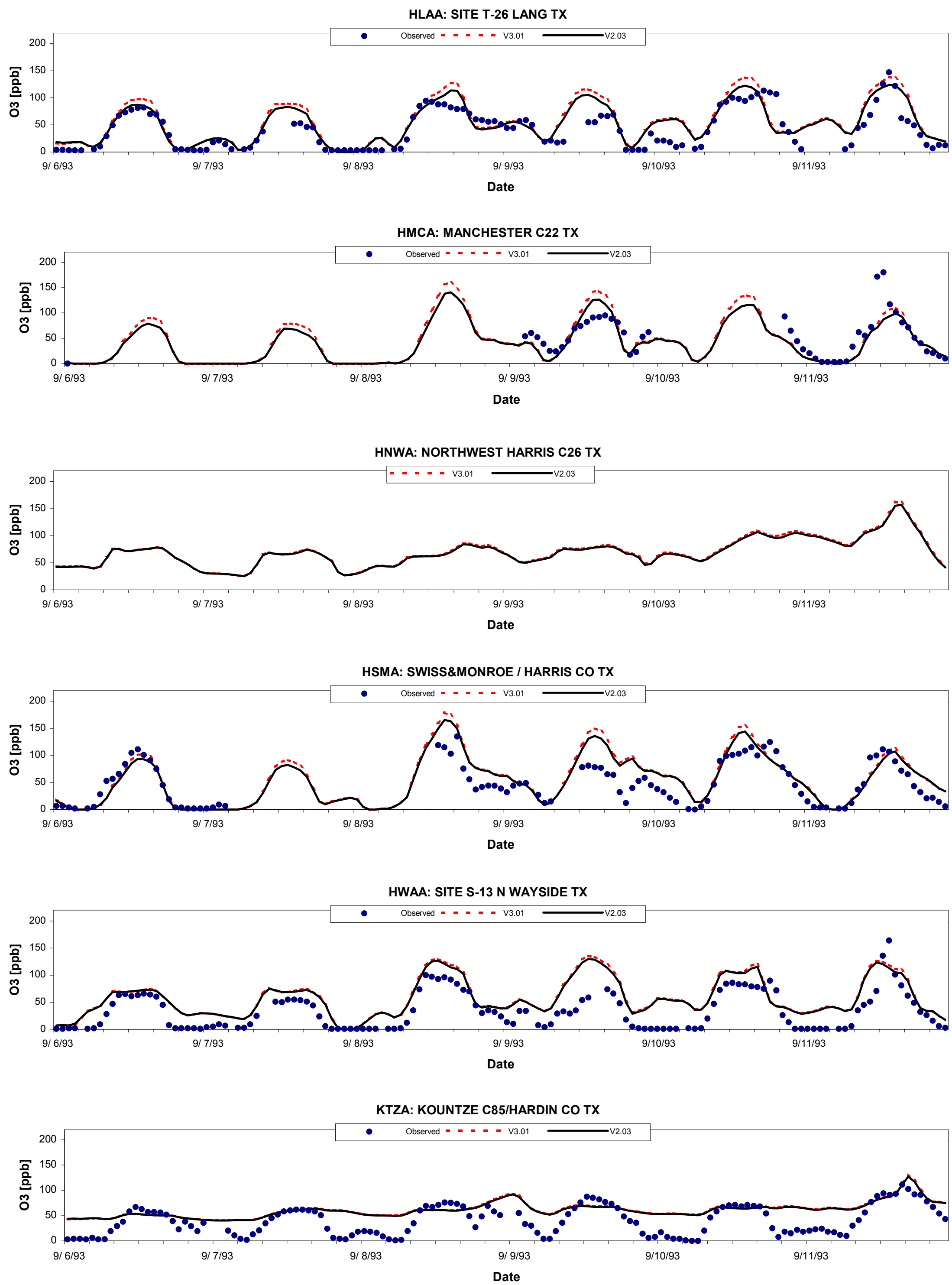


Figure 3-9. (continued).

SuperCOAST September 6-11,1993

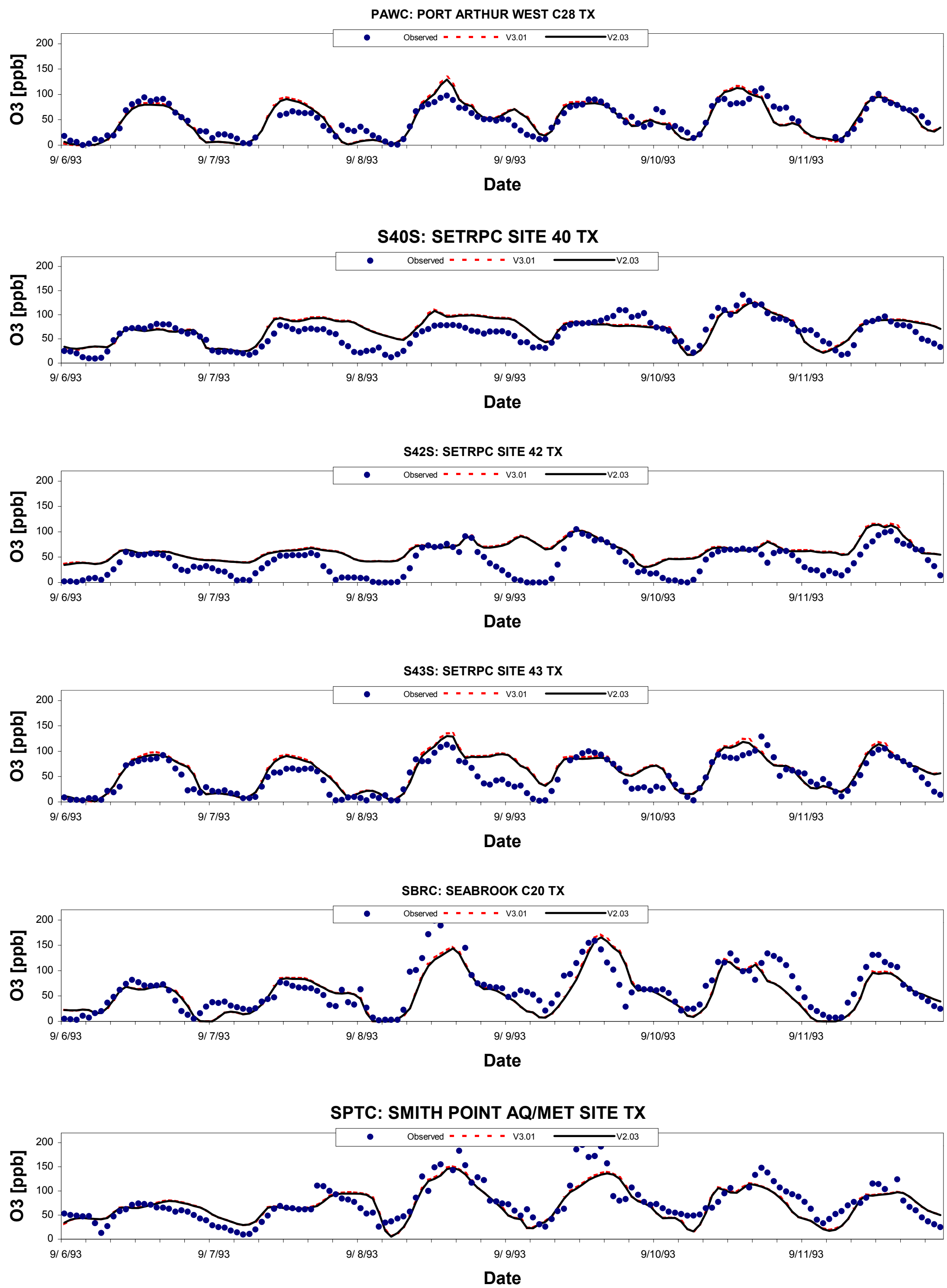


Figure 3-9. (continued).

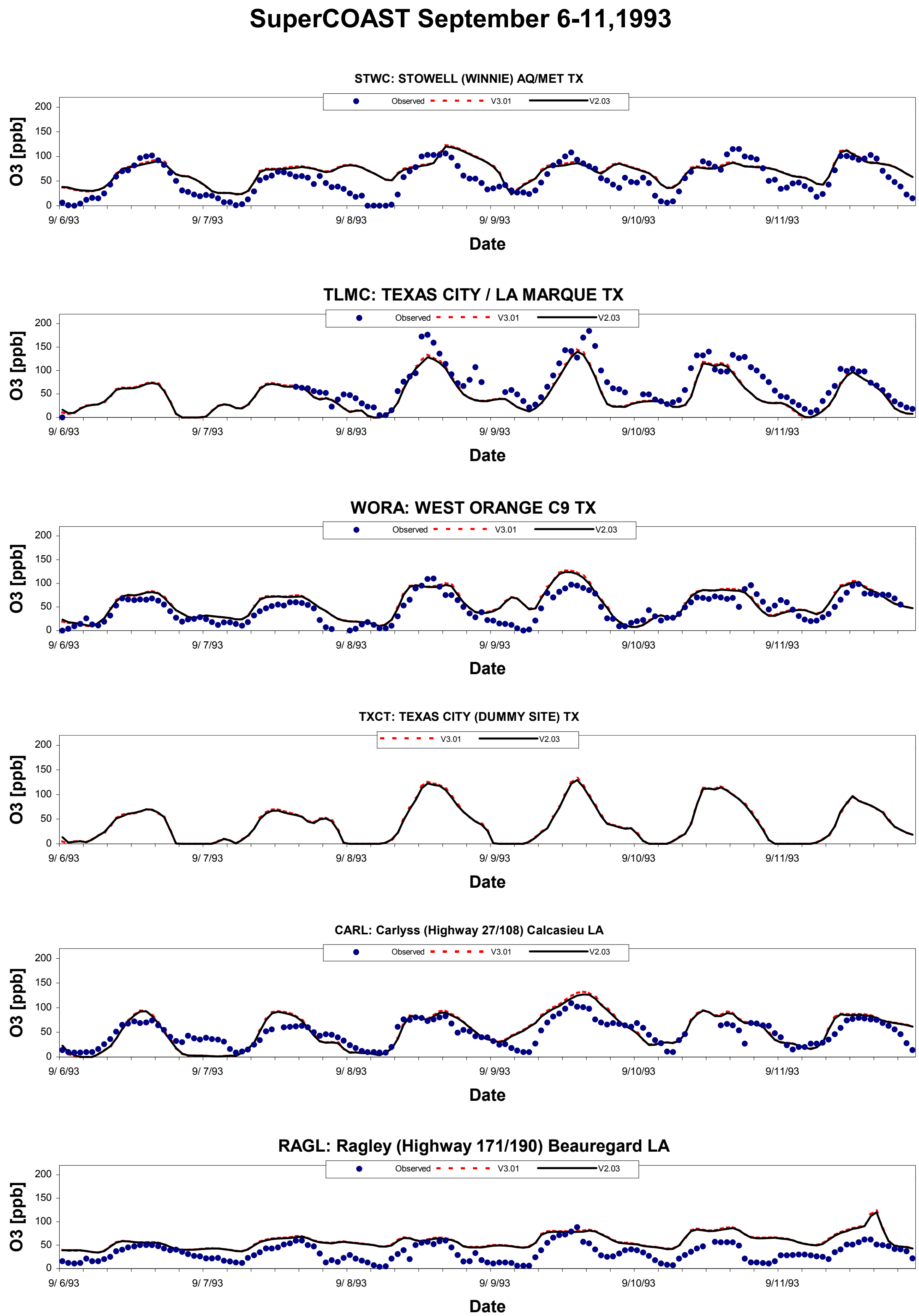


Figure 3-9. (continued).

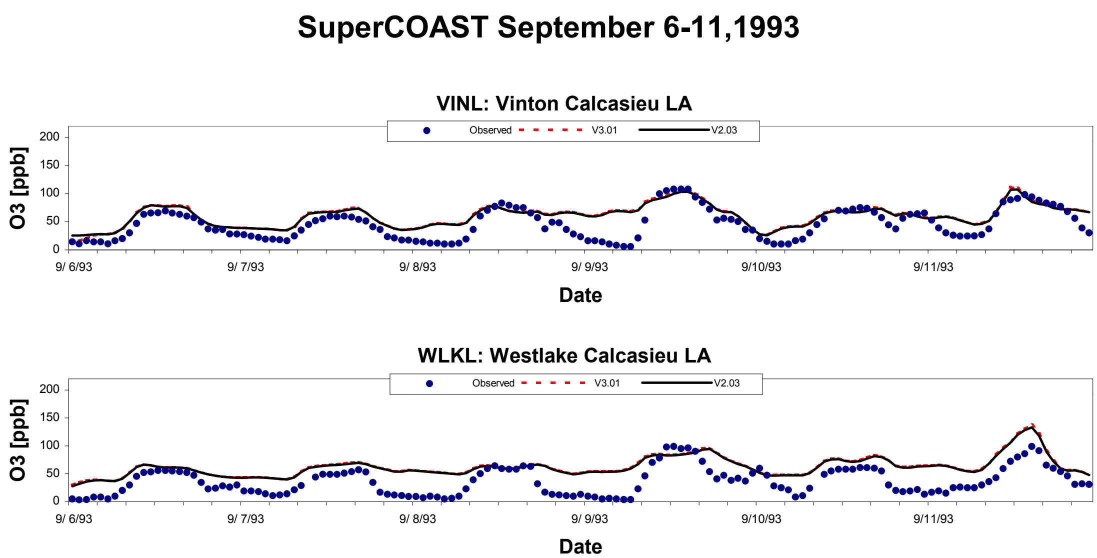


Figure 3-9. (concluded).

SuperCOAST September 6-11,1993

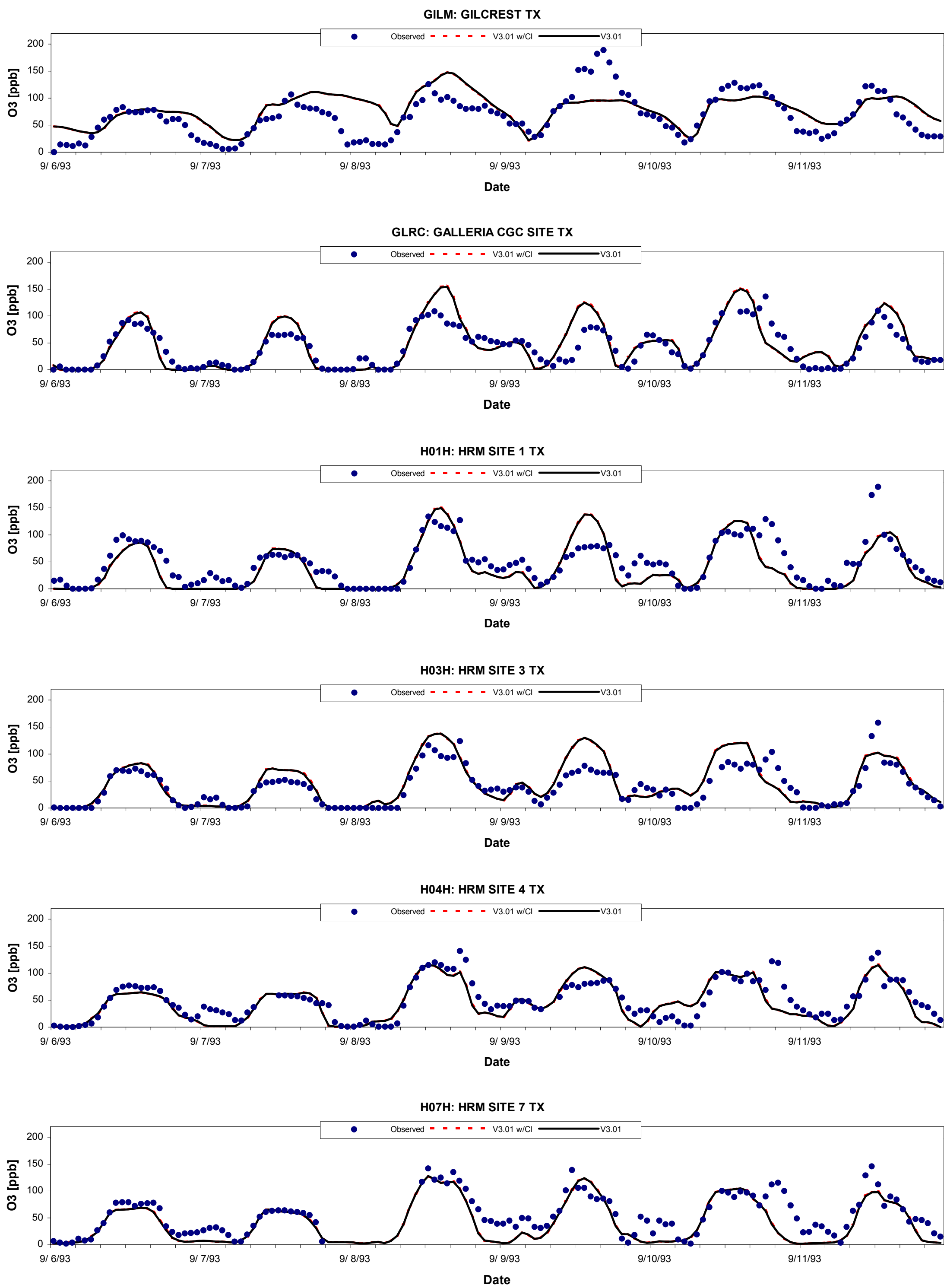


Figure 3-10.

SuperCOAST September 6-11,1993

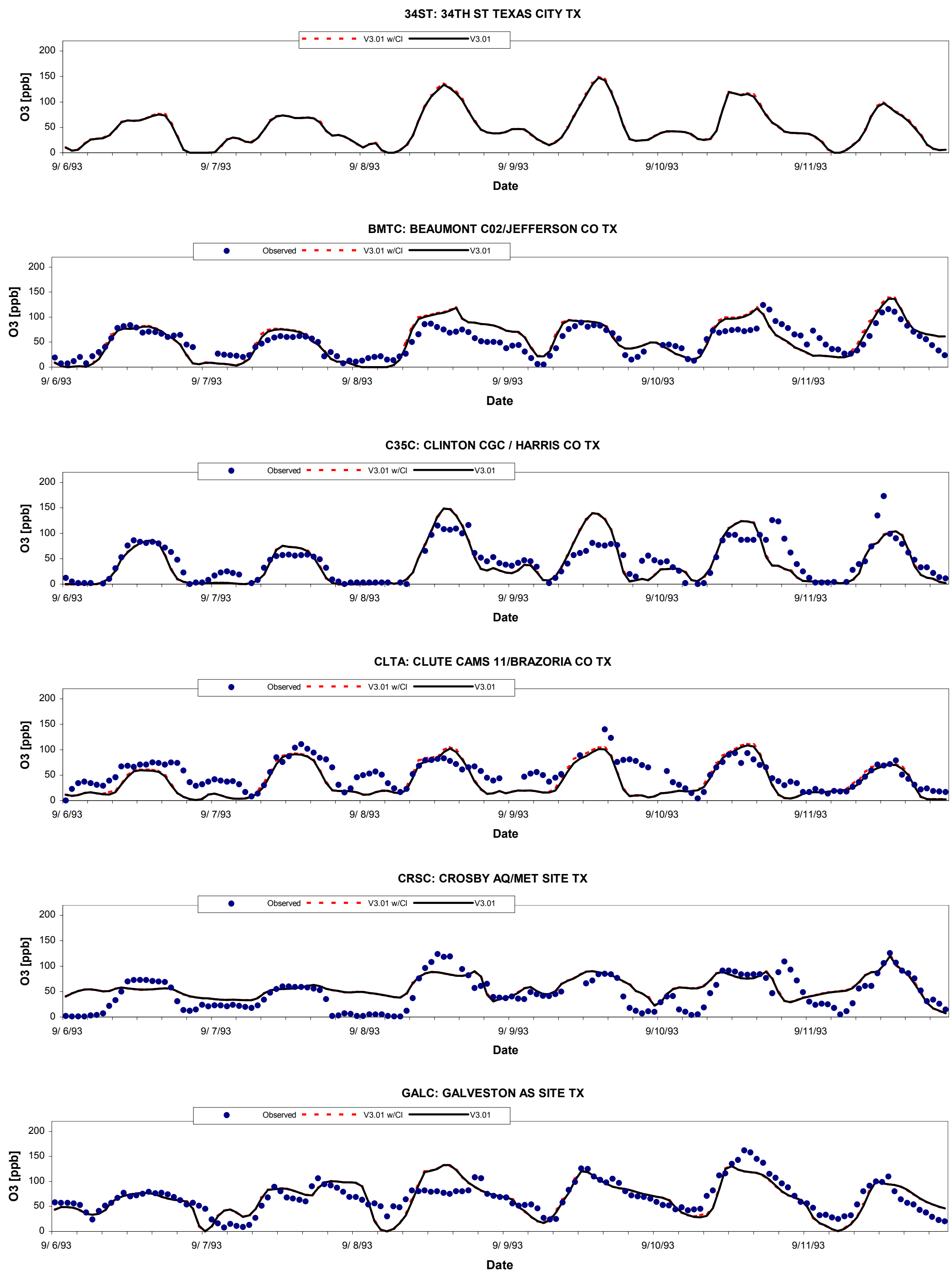


Figure 3-10.(continued)

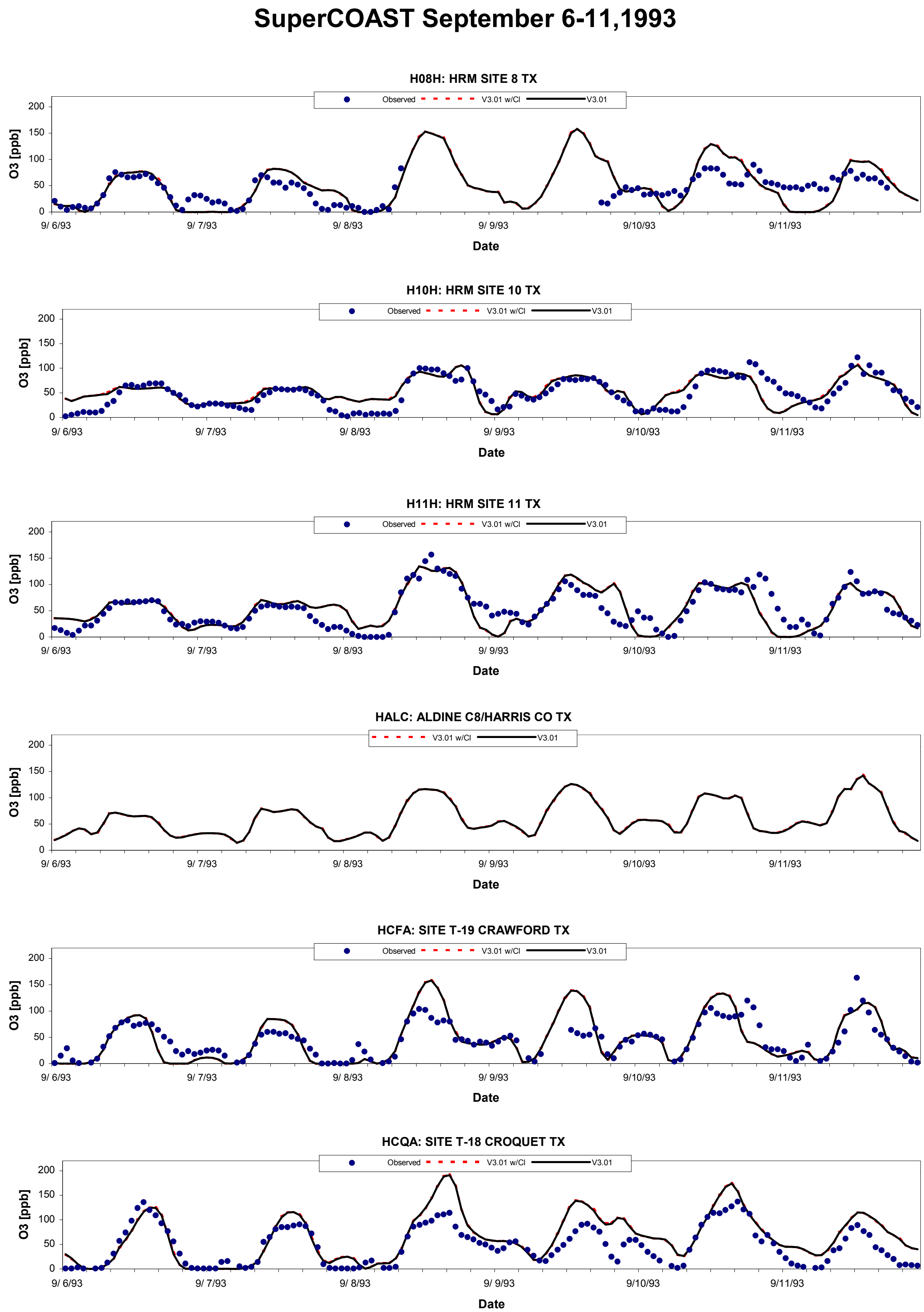


Figure 3-10.(continued)

SuperCOAST September 6-11,1993

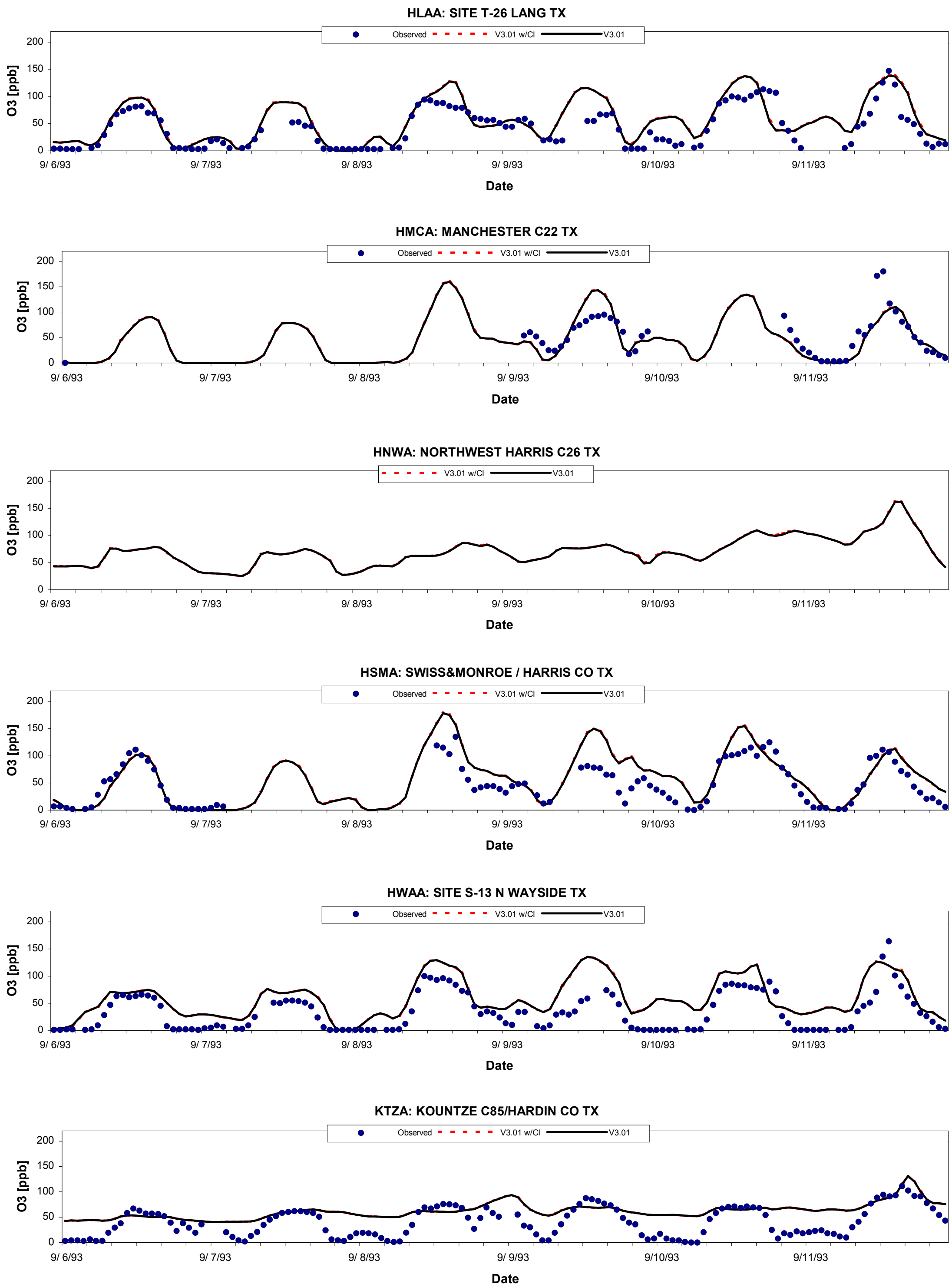


Figure 3-10.(continued)

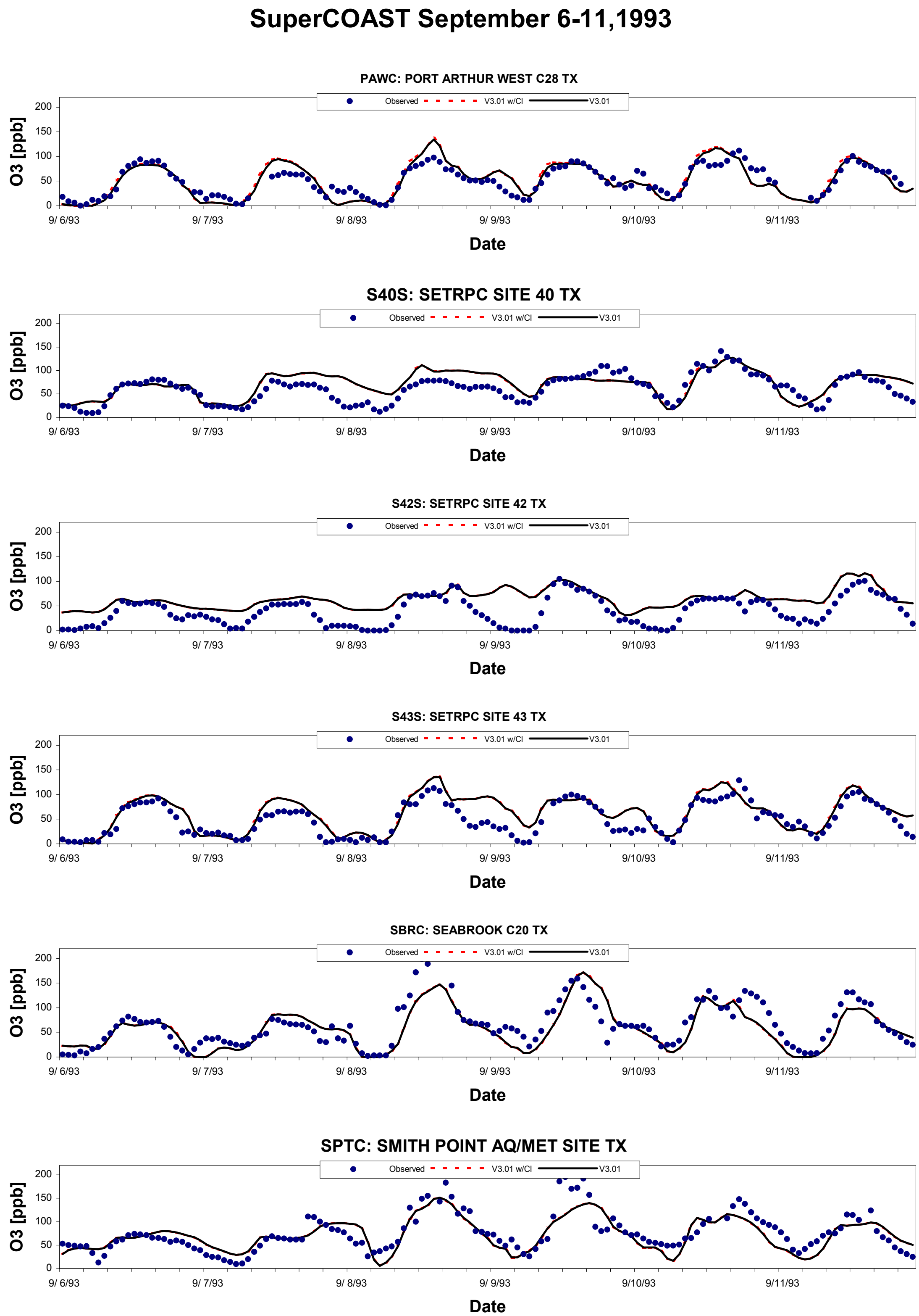


Figure 3-10.(continued).

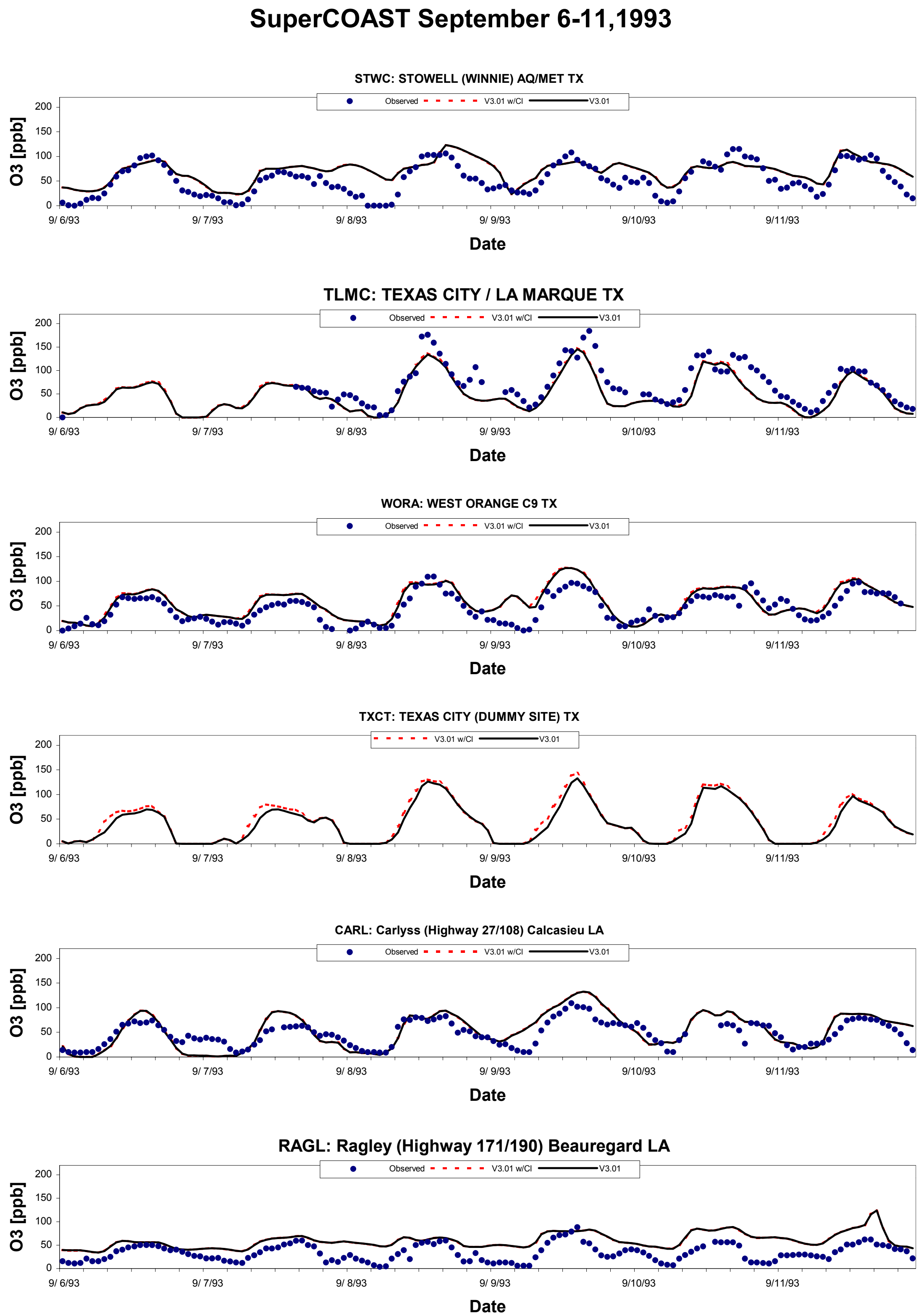
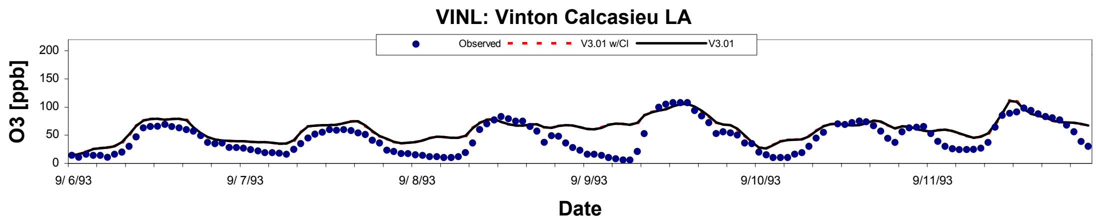


Figure 3-10.(continued)

SuperCOAST September 6-11,1993



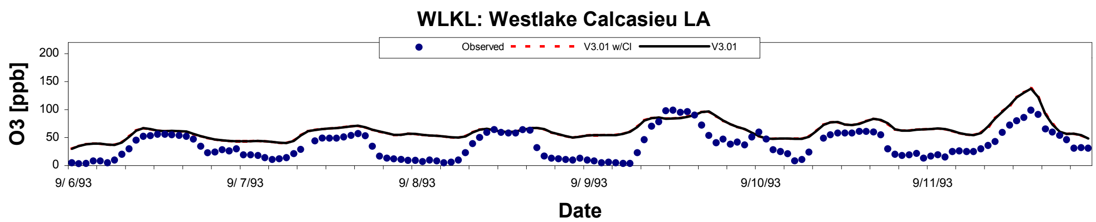


Figure 3-10. (concluded)

SuperCOAST September 6-11, 1993 -- 4-km Grid

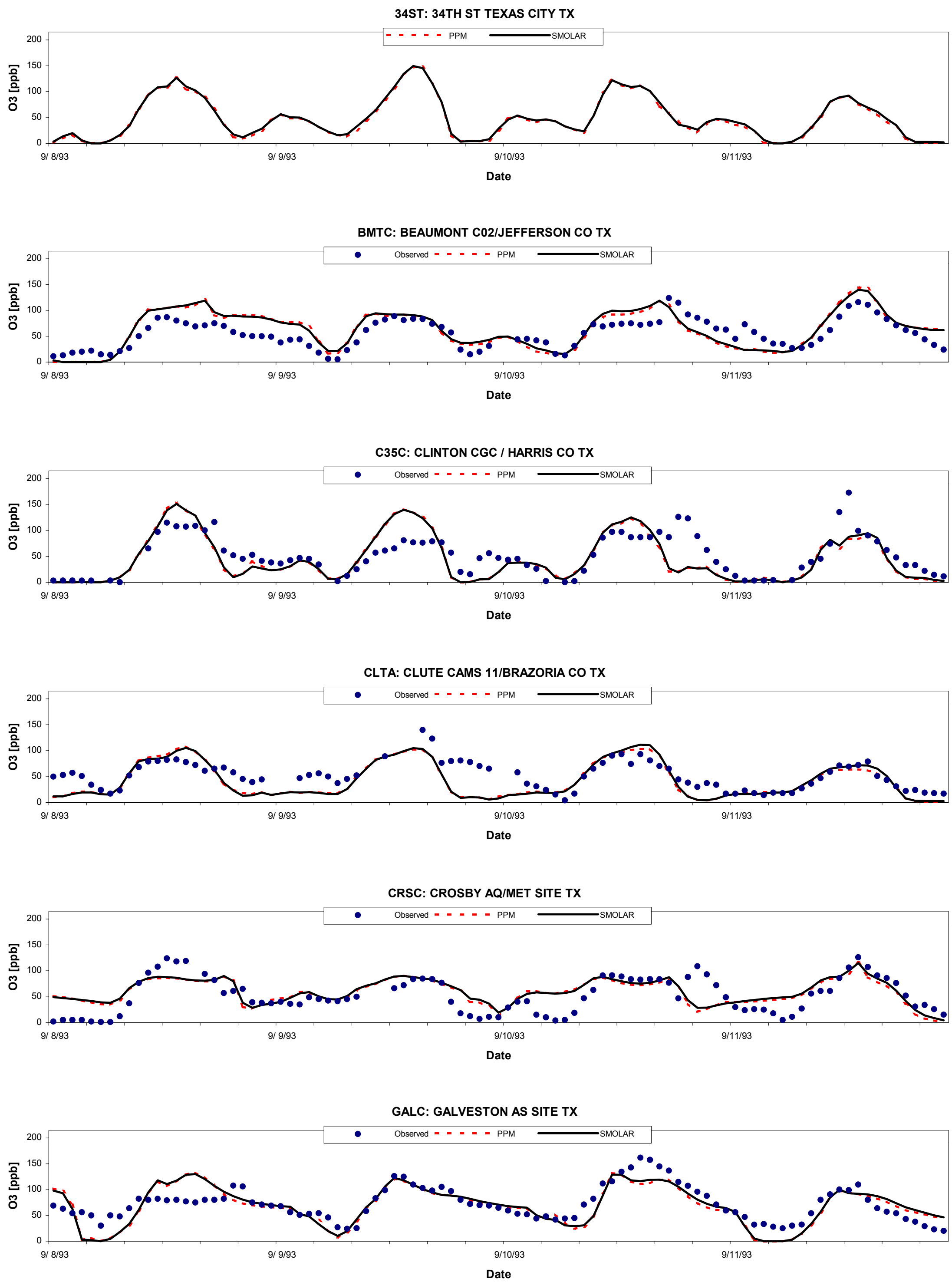


Figure 3-11.

SuperCOAST September 6-11, 1993 -- 4-km Grid

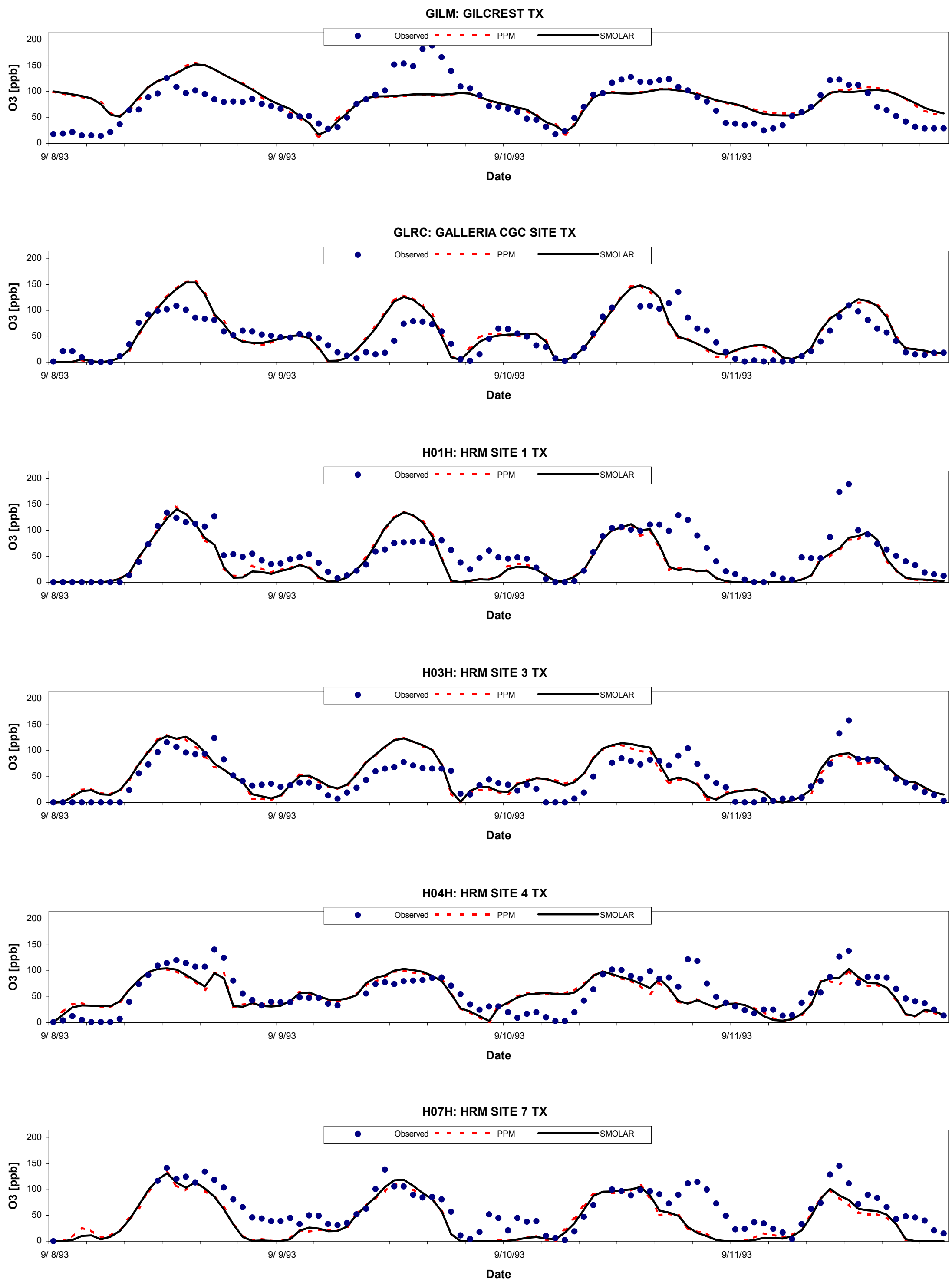


Figure 3-11. (continued)

SuperCOAST September 6-11, 1993 -- 4-km Grid

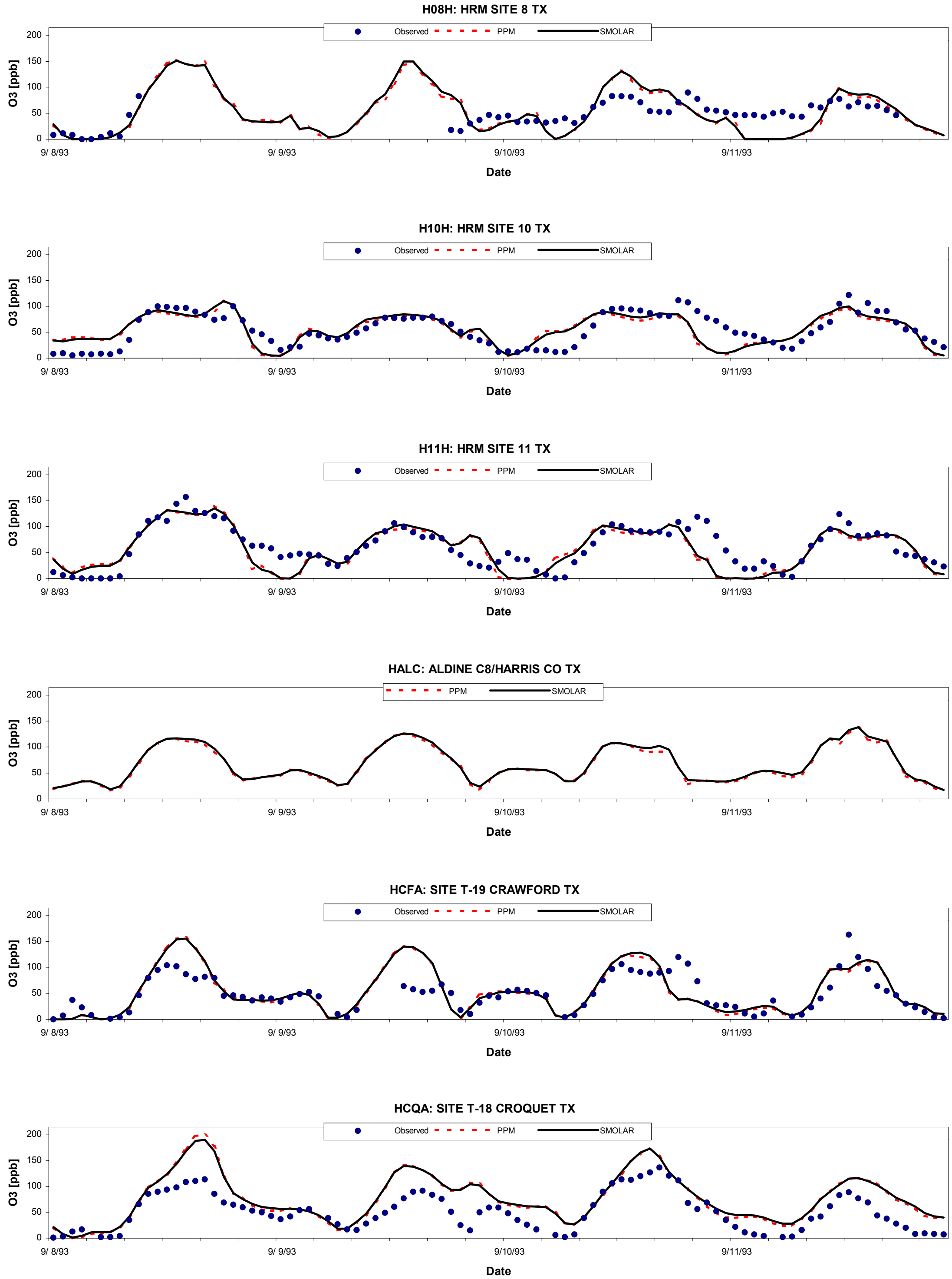
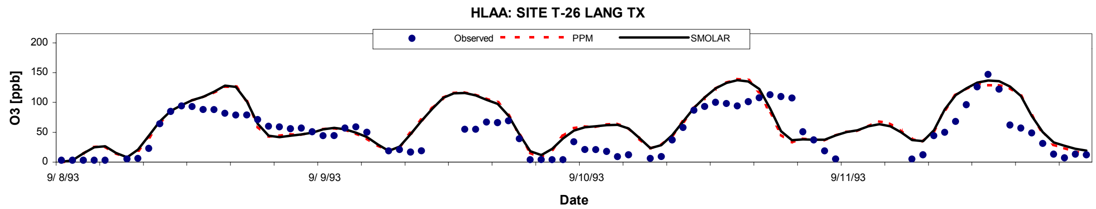
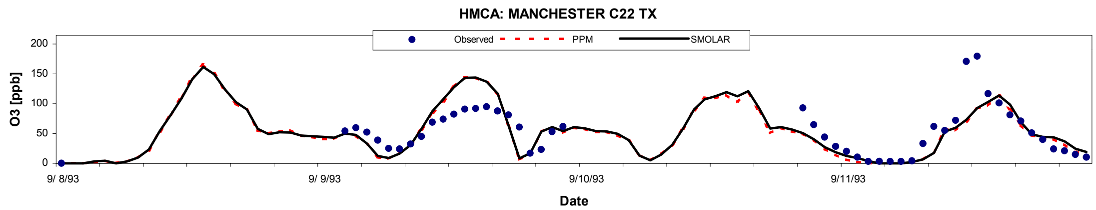
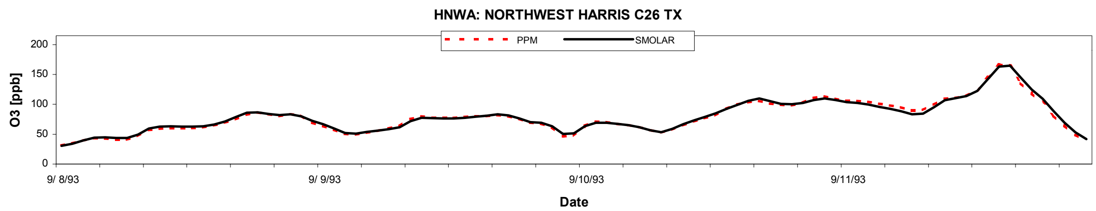


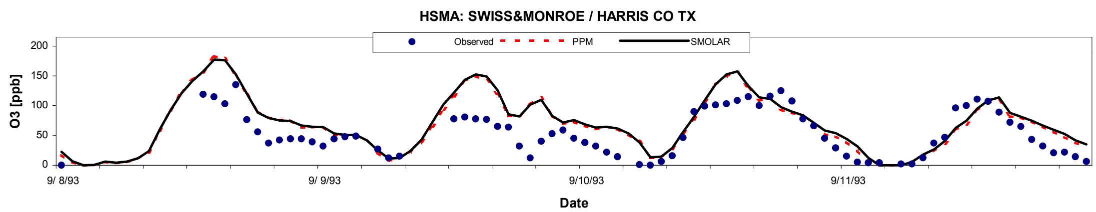
Figure 3-11. (continued)

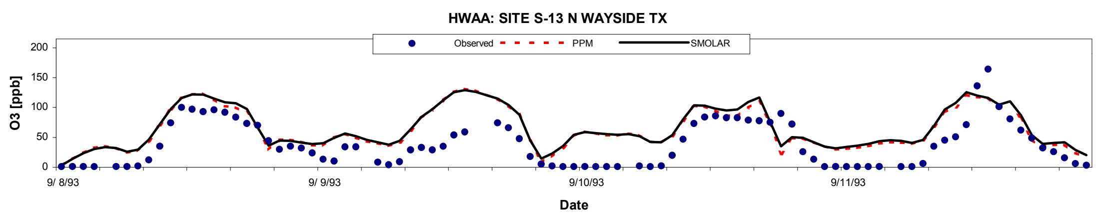
SuperCOAST September 6-11, 1993 -- 4-km Grid











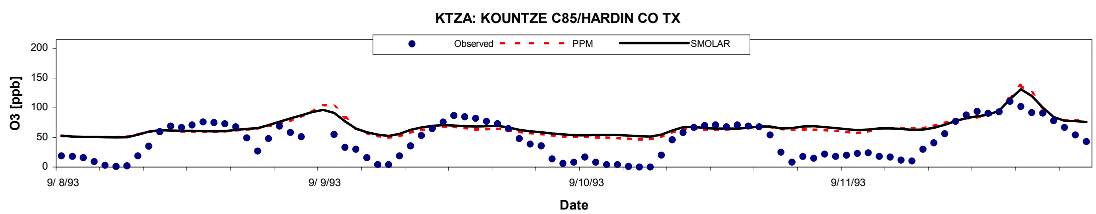


Figure 3-11. (continued)

SuperCOAST September 6-11, 1993 -- 4-km Grid

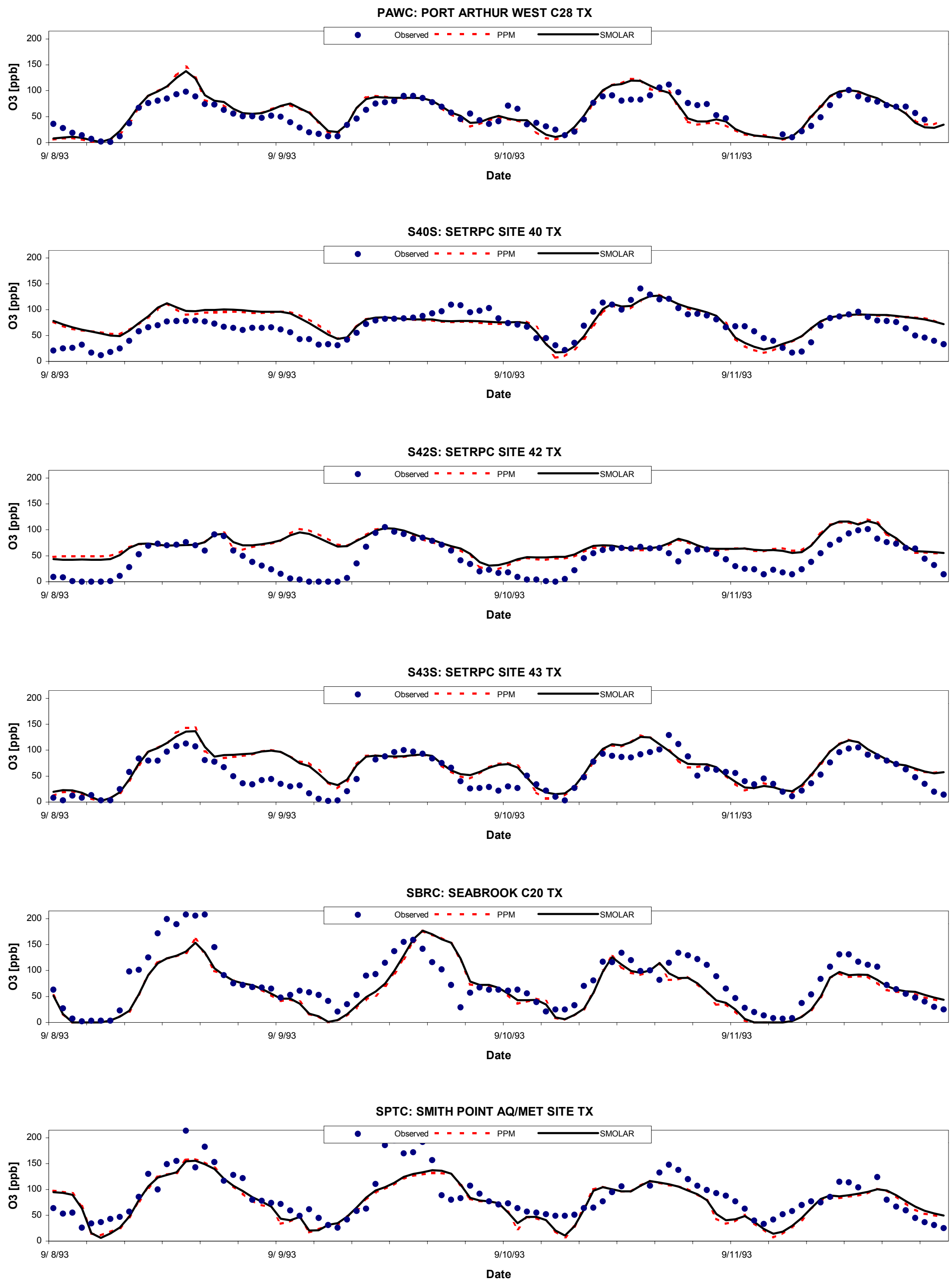


Figure 3-11. (continued)

SuperCOAST September 6-11, 1993 -- 4-km Grid

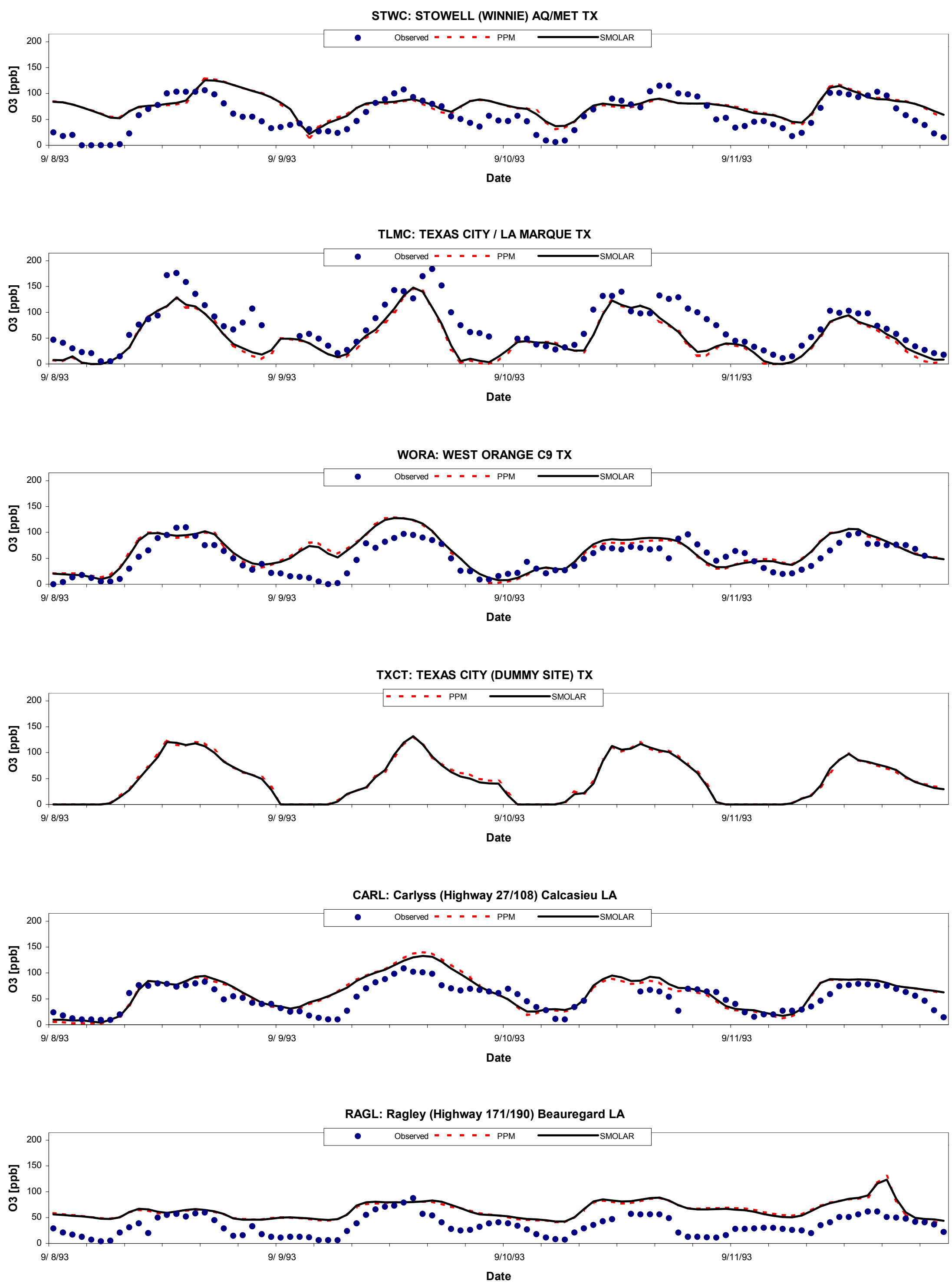
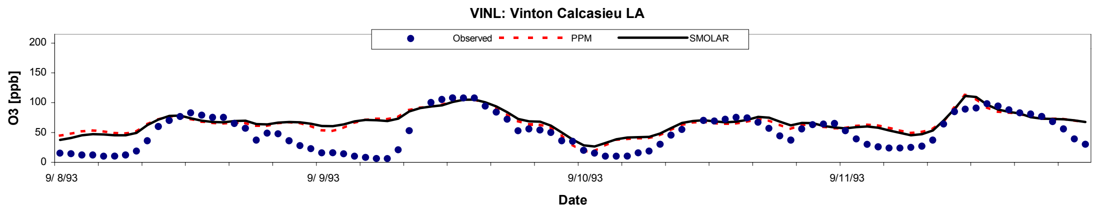


Figure 3-11. (continued)

SuperCOAST September 6-11, 1993 -- 4-km Grid



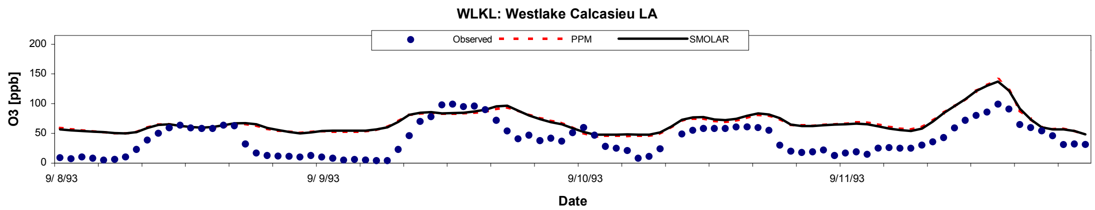


Figure 3-11. (concluded)